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Methodology for Chemical Hazard Prediction

Department of Defense Explosives Safety Board

Alexandria, Virginia

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PREFACE

This document describes an atmospheric-diffusion model which provides an appropriate method for calculating hazard-distances associated with chemical accidents or incidents for emergency-planning purposes. Background, experience, and judgment are required in the responsible employment of these methods. That judgment is required to determine source parameters, to use the meteorological input parameters, and to apply the model to situations involving changing meteorological environments. Integrity of the results obtained will reflect the users' understanding of the physical processes, models, methods and, when utilized, computer programs.

The method described in this Technical Paper is the product of a coordinated effort of Technical Advisors to the Chemical Standards Working Group, DoD Explosives Safety Board. The Technical Advisors were Mr. P. E. Carlson (Dugway Proving Ground), Mr. C. G. Whitacre (Chemical Systems Laboratory, US Army Armament Research and Development Command), Mr. J. D. Wood (US Army Ordnance and Chemical Center and School), Mr. I. Solomon (retired), and Mr. M. C. Johnson (US Army Armament Materiel Readiness Command). In addition, considerable expert advice and support in matters related to meteorology were provided by Dr. H. E. Cramer of H. E. Cramer Company under DPG Contract DAAD09-74-C-0005.

The original Working Group members were:

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The concerted effort exerted by the above named persons is appreciated. It is considered to be a significant advance in the evaluation of the downwind hazards associated with the release of toxic chemical materials.

Change 3 incorporates methodology for agent evaporation in still air. The technical assistance of Headquarters, US Army Armament Materiel Readiness Command in reviewing this change is acknowledged and greatly appreciated.

Alton W. Powell
ALTON W. POWELL
Colonel, USAF
Chairman

June 1980

This Change 3 supersedes the original publication and subsequent changes which should be destroyed.

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CHAPTER 1

INTRODUCTION

1.1. PURPOSE. The purpose of the Technical Paper is to present a description of the current, recommended method for estimating chemical hazard distances for planning purposes.

1.2. SCOPE

This Technical Paper describes an appropriate method for estimating, for planning purposes, hazard distances associated with hypothetical Maximum Credible Events (MCE) from which toxic substances might be released into the atmosphere. In particular, the method comprises a mathematical model, which reflects the current state-of-the-art in atmospheric diffusion modeling, and complete sets of input data representing appropriate parametric values for wide ranges of geographical and meteorological environments. Certain subordinate mathematical models are also provided to facilitate calculations when the MCE includes either spills of toxic substances onto ground surfaces or plumes which ascend rapidly because of heat generated by fuel fires, etc.

Not included in the scope of this Technical Paper are those factors which lead to development and identification of the MCE.

CHAPTER 2

THE RECOMMENDED MODEL

2.1. GENERAL

a. The recommended method for calculating toxic vapor hazard distances for planning purposes, given the agent source configurations, is a Gaussian Plume diffusion model with (a) provisions for limiting the vertical expansion of the cloud to the surface mixing layer and (b) criteria to accommodate time-space variations of meteorological and other environmental factors. The theoretical basis for that model has been extensively investigated and reported by Sutton[1*] and Pasquill[2], among others. Sutton shows that the Gaussian Plume model is a natural consequence of treating atmospheric diffusion as an analogy to molecular diffusion. Diffusion coefficients associated with Brownian motion in the molecular case are simply replaced by those associated with the size of thermally-generated wind eddies in the atmospheric case.

b. Historically, the practical problem has been to determine the rate of diffusion from observations of plume densities (concentrations) and simultaneous measurements of purely meteorological entities, such as wind, temperature, cloud cover and relative humidity. Even, in the simplest case, i.e., flat, level and open terrain free from vegetation and man-made structures, the problem is not an easy one. The presence of hills, vegetation and structures further complicates the practical problem.

A majority of toxic vapor hazard problems can be treated adequately with the Basic Model described below. It is applicable when the ground-level, axial, total dosage is required in an idealized topographic situation (i.e., flat, level and open terrain). Problems which do not fall in this category can be treated via either the more general or more special methods described in the various Annexes to this Technical Paper.

2.2. THE BASIC MODEL

The basic equation for computing the axial dosage at ground level from an elevated, instantaneous, point-source or computing axial concentration at ground level from an elevated, continuous, point-source is:

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* Superscript numerals designate references listed at the end of text.

$$D(x) = \frac{Q}{\pi \sigma_y \sigma_z U_x} \cdot \qquad (2.1)$$

$$\left\{ \exp -1/2 \left(\frac{H}{\sigma_z} \right)^2 + \sum_{i=1}^{\infty} \left[\exp -1/2 \left(\frac{2iH_m + H}{\sigma_z} \right)^2 + \exp -1/2 \left(\frac{2iH_m - H}{\sigma_z} \right)^2 \right] \right\}$$

where:

D = the axial dosage in mg-min/cu m at a point, x, downwind (concentration in mg/cu m for continuous point sources.

Q = the source strength in milligrams (milligrams/min for continuous sources).

σ_y & σ_z = the standard deviations of crosswind and vertical concentrations respectively, in meters. Both are functions of the distance, x.

U_x = the average speed of the cloud as it passes the point x, in meters/min.

H_m = the depth of the surface mixing layer, in meters.

H = the effective height of the source, in meters. (H should not exceed H_m in the above equation).

Equation 2.1 can be approximated by a very simple linear expression,

$$D(x) = \frac{Q}{\sqrt{2\pi}\, \sigma_y H_m U_x}, \qquad (2.2)$$

at moderate distances, x, downwind from the toxic source, where the effect of the release height, H, on the dosage, D(x), becomes negligible. At those distances, the toxic substance becomes rather uniformly distributed in the vertical because of multiple reflections of material from the assumed perfectly-reflecting planes at ground level and at the inversion cap height, H_m. Equation 2.2. is commonly known as the "Box Model." Because of its simplicity, it is preferred over the more complex Equation 2.1. However, in practice, care must be taken to insure that assumptions fundamental to the Basic Model remain valid (see paragraph 3.2, Stability Change Criteria).

The parameters σ_y and σ_z, as used in the Basic Model, are defined as simple power-law functions of the distance traveled by the toxic plume. Values for those parameters at any downwind distance, x, are computed from auxiliary equations, as follows:

where σ_{yr} and σ_{zr} are reference values at the distances x_{yr} and x_{zr}, respectively. Further, α and β are stability-dependent values which describe the expansion rates of the cloud laterally and vertically, respectively. B and C are virtual distances calculated to allow for a volume source and are obtained as follows:

$$\sigma_y = \sigma_y(x) = \sigma_{yr}\left(\frac{x+B}{x_{yr}}\right)^{\alpha} \tag{2.3a}$$

$$\sigma_z = \sigma_z(x) = \sigma_{zr}\left(\frac{x+C}{x_{zr}}\right)^{\beta} \tag{2.3b}$$

Where σ_{yR} and σ_{zR} are the initial values describing the initial size of the toxic plume at the site of the hypothetical accident/incident. Specification of values for the parameters σ_{yR} and σ_{zR} requires a detailed knowledge of the source configuration in terms of toxic substance and its physical state), source strength (Q), time duration of release, and height of the toxic plume's centroid. These elements of the source configuration must necessarily be derived from the hypothetical MCE. They often involve complex technical judgements which are specific to the MCE under study and which will be provided by the agency which conducts the scenario-specific hazard study.

Recommended values for all meteorological variables introduced in the Basic Method have been tabulated. They appear in paragraph 4.2. If, however, calculations are being made for a location for which specific meteorological data are available, those data should be used in lieu of the data in paragraph 4.2.

2.3. A GENERALIZED MODEL. The mathematical formulation of a generalized model is presented in Annex A. The generalized model provides for variations in the composition and quantity of the material released, as well as for variations in source dimensions, source height, source emission time, and decay. Specific provision is also made in the generalized model for the effects of gravitational settling and for computing dosages and concentrations for locations other than downwind plume centerlines, at ground level. That model will also accommodate the restriction of lateral diffusion due to orographic influences of terrain channeling. Meteorological model inputs include mean wind speed, depth of the surface mixing layer, intensities of turbulence, and vertical shear (i.e., wind direction and wind speed) in the mixing layer. Thus, the generalized model contains both mesoscale and microscale meteorological predictors that may be tailored to specific geographical locations and specific meteorological conditions.

CHAPTER 3

SPECIAL CONSIDERATIONS

3.1. GENERAL. Four special considerations have been identified as necessary, on occasion, in the application of the Basic Method to toxic hazard predictions. These are (1) stability-change criteria, (2) personnel exposure times, (3) the rates of evaporation from spill s of toxic substances, and (4) the extent of vertical rise of heated plumes which are generated by the heat released from fuel fires, etc.

3.2. STABILITY CHANGE CRITERIA

The recommended Basic Model, and its implementation in terms of formulas given above, computer programs, and parameter values shown in paragraph 4, is based on the assumption that steady-state conditions exist throughout the air volume swept out by the toxic plume during its lifetime. That volume might exceed billions of cubic meters (i.e., during its lifetime, the plume might occupy air volumes whose dimensions are several kilometers in the vertical and lateral, and hundreds of kilometers extending downwind from the plume's source). Lifetimes of large, dense plumes could reach tens or hundreds of hours. In many instances, the assumption that steady-state conditions exist over those volumes and those time intervals simply fails: Even if surface properties of the local terrain are uniform enough, over large land areas, to suggest steady-state atmospheres, the normal diurnal changes would preclude maintenance of the steady-state after several hours have elapsed. This situation typically occurs when large amounts of toxic material are released during a very stable nighttime regime with very low wind speeds and mixing depths. The maximum time-duration of a stable nighttime regime is generally 12 hours or less, depending on the season of the year and the latitude.

Techniques have been developed to accommodate these dynamics within the current, recommended Basic Model. The concept is as follows: Although it is recognized that transitions in the atmospheric structure occur smoothly, they are treated as a series of discrete step-changes. The computer-assisted calculations are interrupted at "appropriate" points in the process, final calculated values of the plume variables recorded, and these final values are treated as initial values in the next subsequent phase of the calculation. The "appropriate"" points in the process are where the analyst has reason to believe that the atmospheric structure would have changed enough to warrant its approximation as a discreet step-change. Thus, some judgement is required.

In the case of the stable nighttime regime cited above, the step-change procedure would be to progressively change the meteorological parameters, which represent the stability categories, from stable to less stable, permitting a reasonable time of dwell in each category. During each phase of the calculations, the axial dosages at downwind distances would be calculated via the Box Model (Equation 2.2), where:

$$H_m = H_{mc} + \frac{\Delta H_m}{\Delta t} \cdot \frac{(x - x_c)}{U_x} \text{ for } H_{mc} \leq H_m \leq H_{mc} + \Delta H_m \tag{3.1}$$

$$\sigma_y = \sigma_{yr} \left(\frac{x + B_c}{x_{yr}} \right)^{\alpha}$$

H_{mc} = the depth of the surface inversion layer at the beginning of the change (m).

x_c = location of the plume's centroid at the beginning of the change (m).

σ_{yr} & x_{yr} = the reference sigma and reference distance in the new stability category (m).

ΔH_m = change in H_m over the interval (m)

Δt = time interval of change (min).

U & α = new meteorological parameters.

$$B_c = x_{yr} \left(\frac{\sigma_{yc}}{\sigma_{yr}} \right)^{1/\alpha} - x_c$$

σ_{yc} = the lateral sigma at the beginning of the change interval.

Where accuracy demands it, and where available resources and technical data input accuracies permit it, the number of discrete steps used to simulate a gradual change in atmospheric conditions could be increased to improve the validity of the approximation. Thus, these techniques can account for the effects of changes in atmospheric stability on the concentration, dosages and deposition patterns of toxic plumes. Normal procedures are used to calculate 1% casualty estimates from that information.

3.3. PERSONNEL EXPOSURE TIMES. Special methods can be used when specific elements of the hazard analysis require consideration of the time interval during which personnel might be exposed to airborne chemical agents. Those situations normally arise when personnel are assumed to be exposed to very low concentrations of agent over extended periods of time such that detoxification of agent occurs within their bodies. Under those circumstances, the Basic Model would yield overestimates of hazard distances. However, appropriate modifications have been made to the Basic Model to adapt it for use in those instances. The resultant, recommended model, an extension of the Basic Model, is described in Annex B.

3.4. EVAPORATION FROM LIQUID SPILLS

Some MCE's provide for spills of toxic materials onto ground surfaces. Toxic vapor plumes are formed when the spilled material evaporates from those surfaces. Evaporation begins when the toxic material is spilled, and it is assumed to continue until the toxic "puddle" has been covered, decontaminated, or until all toxic material has evaporated. The plume, thus formed, is assumed to have been generated from a "continuous source" of toxic material.

The Basic Model for toxic hazard estimation can be applied to the MCE for liquid spills by the proper selection of parameter values: D(x) in Equation 2.1 is interpreted as concentration of toxic substance in the plume, $3\sigma_y r$ is assumed equal to the width of the puddle, and Q is interpreted as the rate of generation of toxic vapors (i.e., rate of evaporation of the toxic substance from the puddle). In order to provide a basis for estimating evaporation rates from a continum of puddle sizes and a variety of wind speed (to include still air), and air temperature combinations, six graphs are presented in Figures 1 through 6 for GB, VX and HD, respectively. In the event that the MCE involves toxic substances other than these three common chemical warfare agents, or the required values are out of the range of values provided by these graphs, the general methods for calculating evaporation rates under either a variety of wind speeds or in still air can be used as indicated in Annex C.

3.5. RISE OF HEATED PLUMES

3.5.1. General

Toxic substances released in association with a fire or an explosion will usually rise as a heated plume which entrains air until an equilibrium with ambient conditions is reached. Thus, the effective source height, H, will be equal to the height attained as a result of buoyant rise z_m.

The formulas given in this section, for instantaneous sources (explosions) and quasi-continuous sources (fires or multiple explosions), are based on procedures similar to those contained in a paper presented by Briggs (1970) at the Second International Clean Air Congress.[3] Briggs' equations differ in form for stable and adiabatic or unstable conditions. The form proposed for adiabatic or unstable conditions contains the time of plume rise as an input value. Since observed values of this parameter are not presently available, practical use of the methodology is limited to the relation proposed for the stable atmosphere, for which this parameter is not required. The equation is stated as a function of the vertical potential temperature gradient and, thus, can be applied from stable to adiabatic.

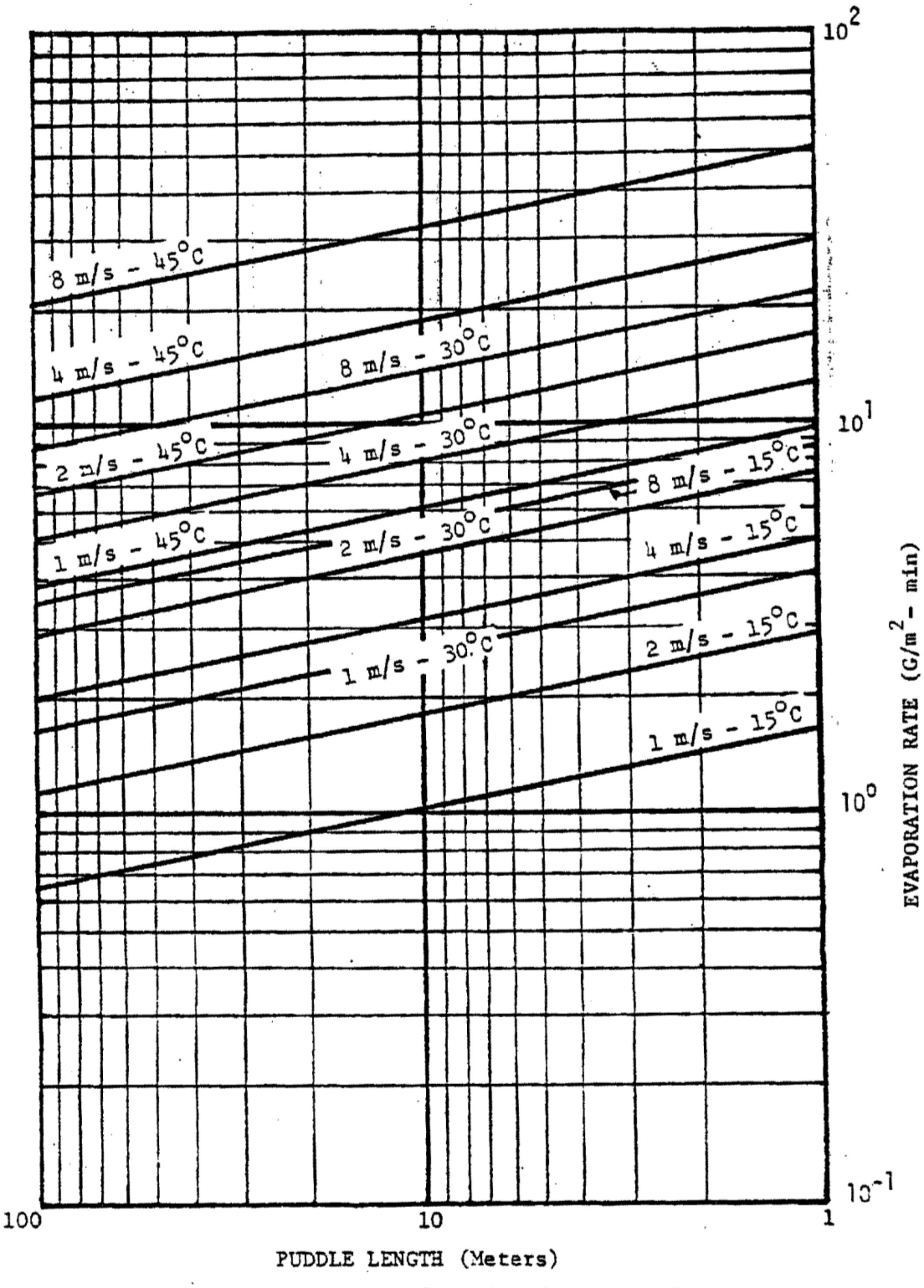

Figure 1: Evaporation Rates for Liquid Spills of GB
with Various Wind Speeds and Air Temperatures

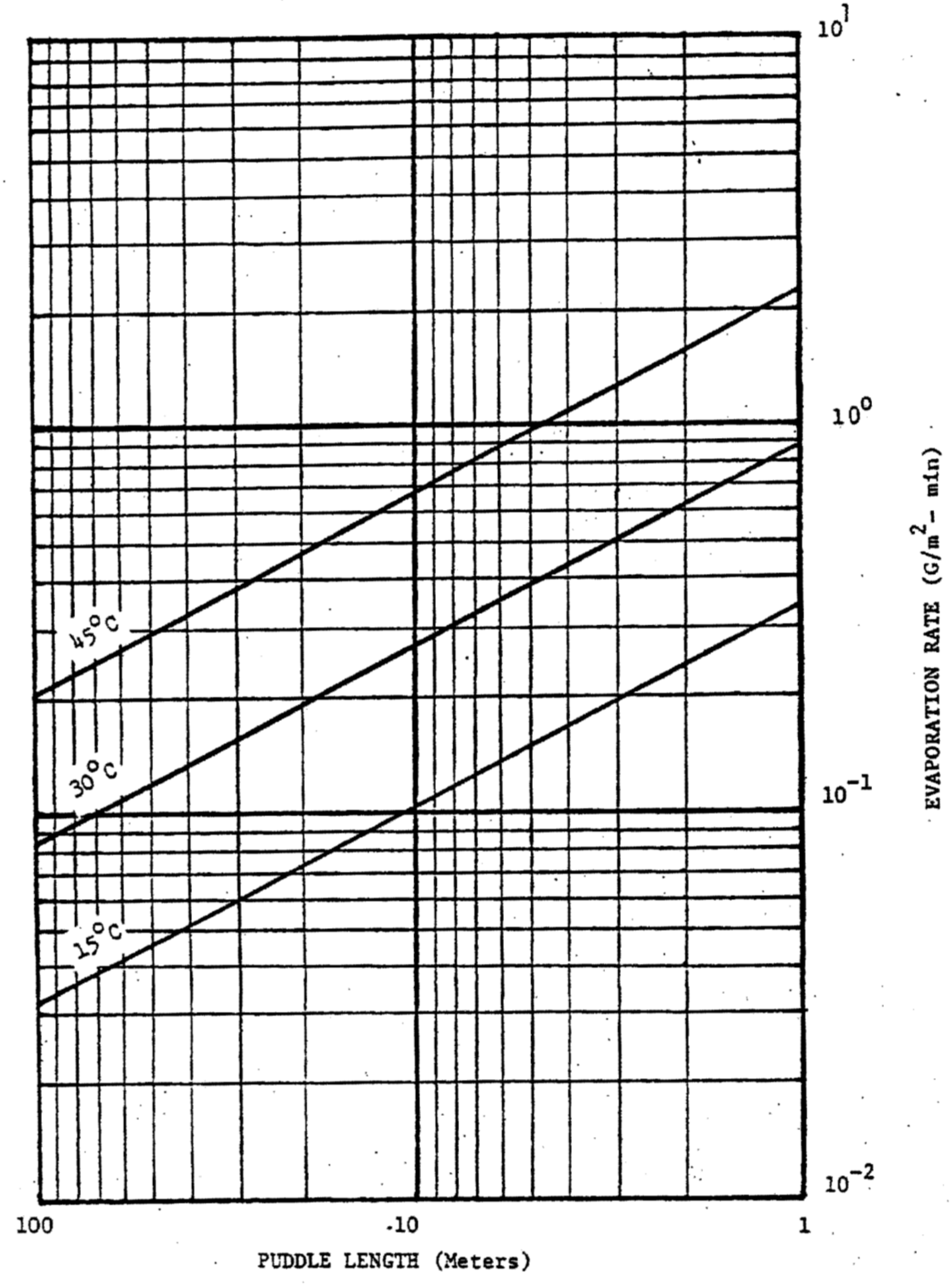

Figure 2: Evaporation Rates for Liquid Spills of GB
in Still Air with a Variety of Air Temperatures

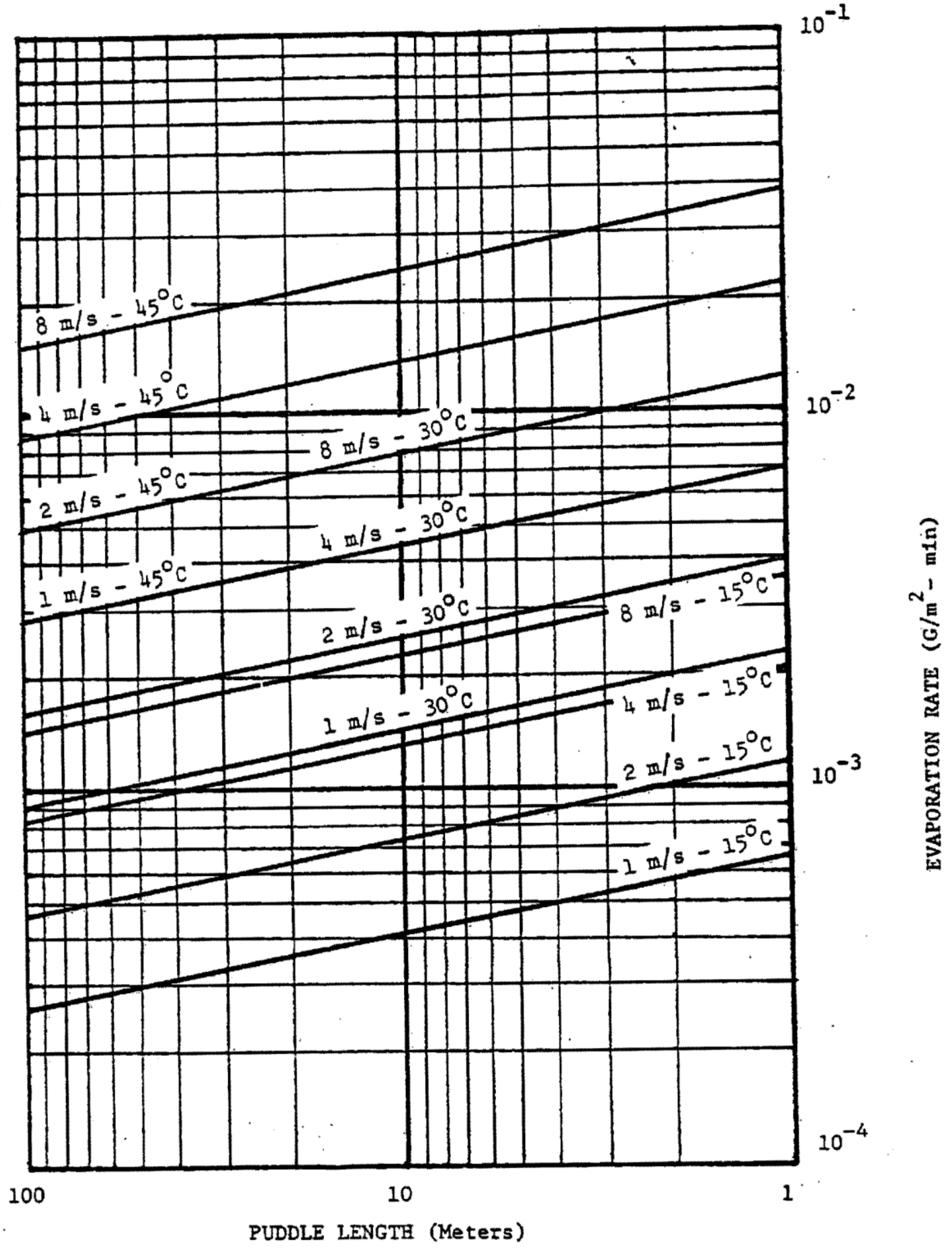

Figure 3: Evaporation Rates for Liquid Spills of VX
with Various Wind Speeds and Air Temperatures

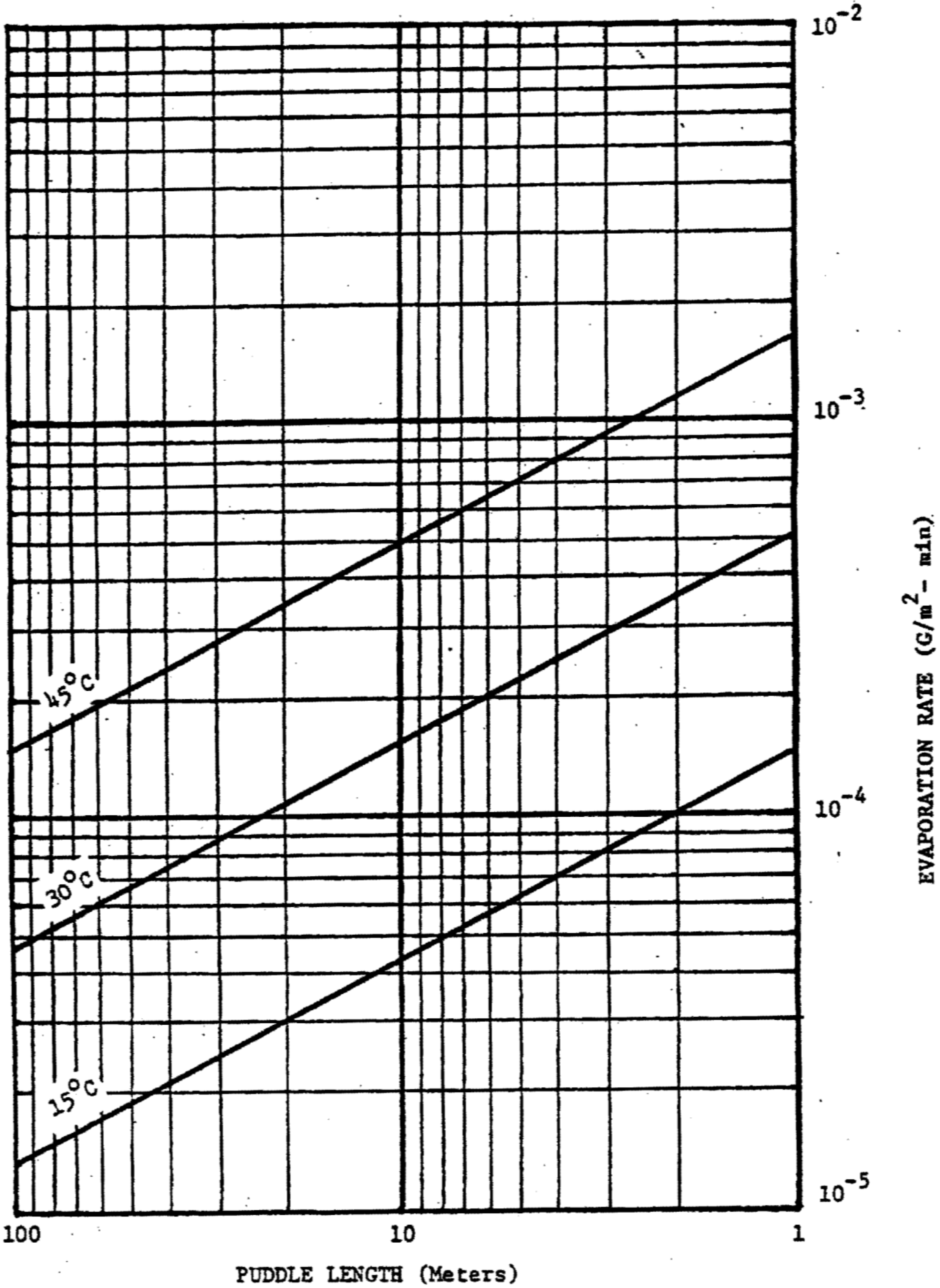

Figure 4: Evaporation Rates for Liquid Spills of VX
in Still Air with a Variety of Air Temperatures

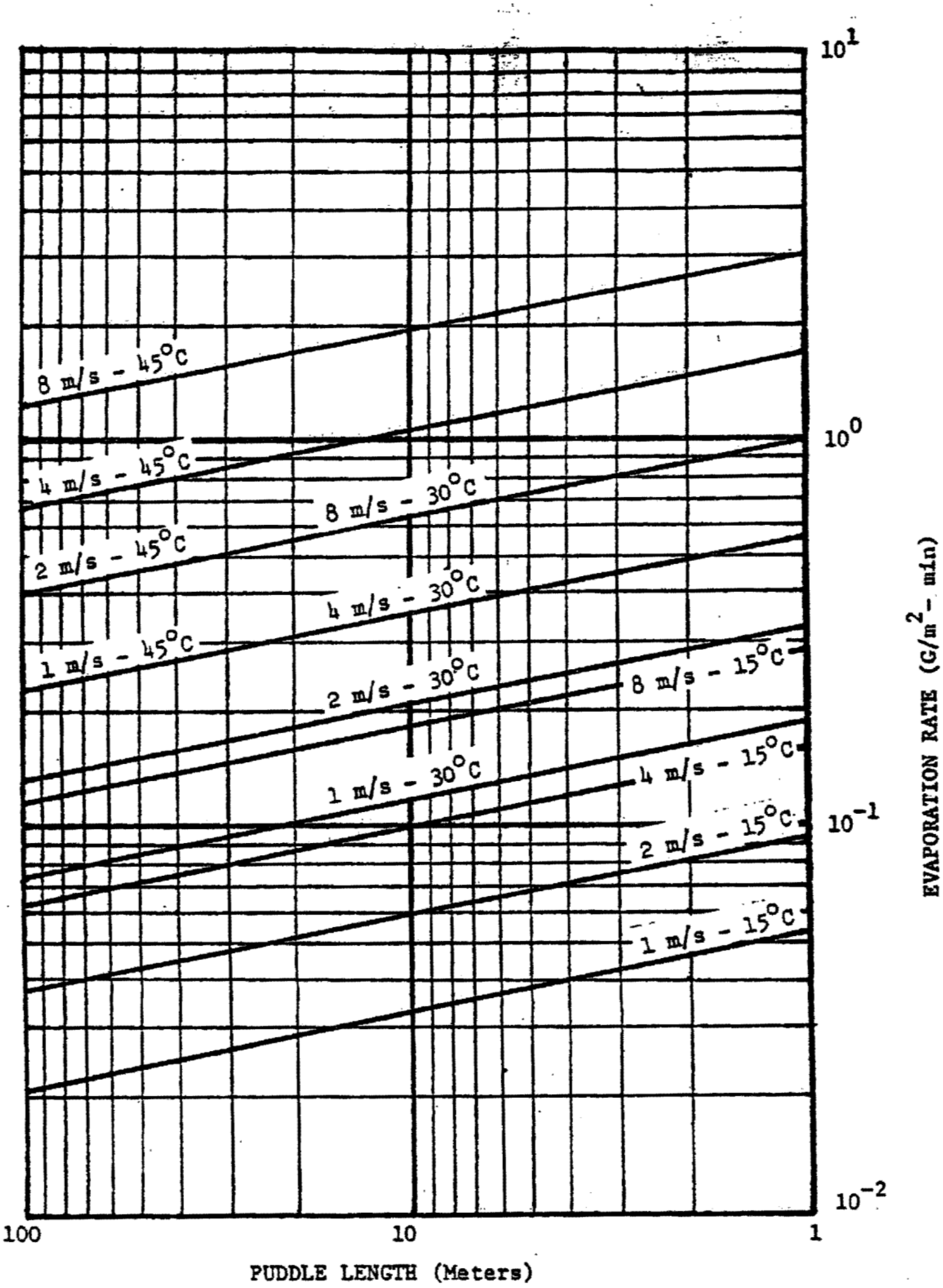

Figure 5: Evaporation Rates for Liquid Spills of HD
with Various Wind Speeds and Air Temperatures

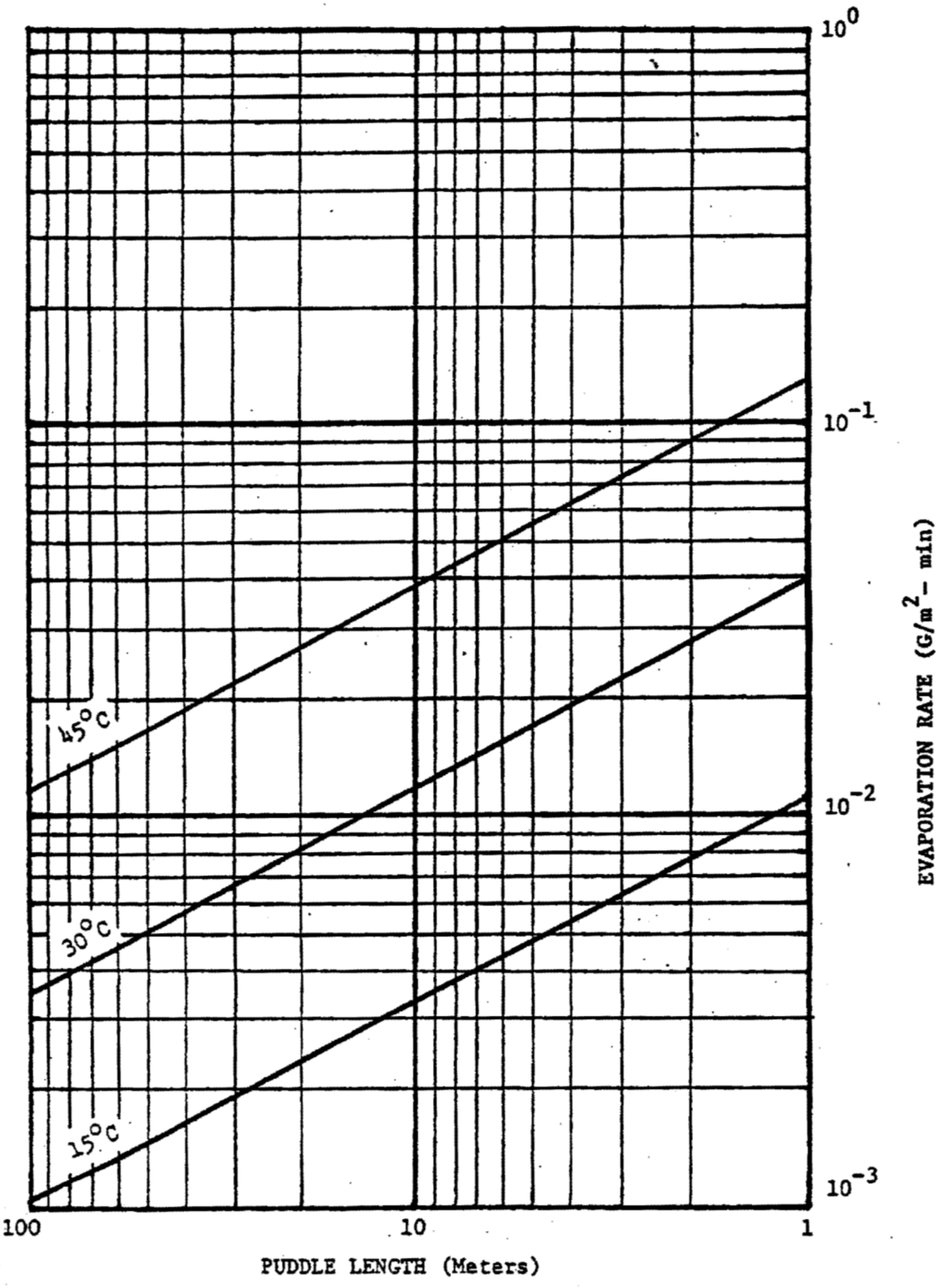

Figure 6: Evaporation Rates for Liquid Spills of HD
in Still Air with a Variety of Air Temperatures

3.5.2. Instantaneous Releases in Stable Atmospheres

The maximum plume rise z_{mL} downwind from an instantaneous source in a stable atmosphere is given by:

$$z_{mI} = \left[\frac{8F_I}{(\gamma_I)^3 s} + \left(\frac{r_R}{\gamma_I} \right)^4 \right]^{1/4} - \frac{r_R}{\gamma_I} \qquad (3.2)$$

where

F_I = the instantaneous buoyancy parameter

$= \frac{3g\,Q_I}{4\,\pi\,\rho_a\,c_p\,T_a}$

Q_I = the effective heat released (cal)

c_p = the specific heat of air at constant pressure (0.24 cal gm^{-1} $^oK^{-1}$)

ρ_a = the density of ambient air (gm per cubic meter)

γ_I = the entrainment coefficient for an instantaneous source

r_R = the initial cloud radius at the surface (m)

g = acceleration due to gravity (9.8 m sec^{-2})

T_a = ambient air temperature (^oK)

$s = \frac{g}{T_a} \frac{\partial\theta}{\partial z} \simeq \frac{g}{T_a} \frac{(\theta_2 - \theta_1)}{(z_2 - z_1)}$

$\frac{\partial\theta}{\partial z}$ = the vertical potential temperature gradient (^oK m^{-1})

θ = the potential temperature at height z

An analysis of time-sequence photographs of the behavior of the ground plumes generated during launches of the Titan I11 D vehicle at Vandenberg Air Force Base[4] suggests that the value of the instantaneous entrainment coefficient, Y_I, may range from about 0.5 to 0.7.

3.5.3. Quasi-Continuous Releases in Stable Atmospheres. The maximum plume rise z_{mc} downwind from a quasi-continuous source in a stable atmosphere is given by:

$$z_{mc} = \left[\frac{6\ F_c}{\bar{U}\ \gamma_c^2\ s} + \left(\frac{r_R}{\gamma_c} \right)^3 \right]^{1/3} - \frac{r_R}{\gamma_c} \qquad (3.3)$$

where

F_c = the quasi-continuous buoyancy parameter

$= \dfrac{g\ Q_c}{\pi \rho_a\ c_p\ T_a}$

γ_c = the entrainment coefficient for a quasi-continuous source

and $\bar{U}$ = the mean wind speed (m sec^{-1})

Plume rise for launches of liquid-fueled rockets and for static firings suggests that the entrainment coefficient γ_c is approximately equal to 0.5.

CHAPTER 4

SUPPORTING DATA

4.1. GENERAL. Two types of supporting data are required in the application of the models to the prediction of hazard distances from chemical accidents/incidents. These data are related to the choices of meteorological parameters and toxicity data to be used in the calculations. Tables of recommended meteorological parameters, together with some justification for their selection, are presented in paragraph 4.2. Recommended values for toxicity of chemical agents at the “1% lethality” for lethal agents and “l% incapacitation” for incapacitating agents are presented in paragraph 4.3.

4.2. METEOROLOGICAL PARAMETERS

Meteorological inputs required for use in the Basic Model are listed below. The specification of numerical values for the meteorological inputs requires, in principle, a complete knowledge of the atmospheric structure of the air volume in which the plume is transported. Because of the large distance scales and the large air volume that may be swept out by toxic plumes, the measurement and specification of representative meteorological inputs is difficult. Thus, it is usually necessary to estimate the requisite meteorological parameters, for any given location, from historical surface meteorological observations, using various approximate techniques based on theory and previous measurements. That has been done for the eleven Army storage depots where chemical material is stored. Those data are presented in Appendix D of the “Handbook for Chemical Hazard Prediction”.[5]

To facilitate hazard distance calculations, the required parameters have been presented for each class of the Pasquill stability categories. The six categories are denoted by the letters A through E. Categories A, B and C represent decreasing degrees of instability; E and F represent increasing degrees of stability; and D is neutral. A summary table relating the stability categories to atmospheric observeables, i.e., solar radiation and wind speed, is presented as Table 1; it has been adapted from Pasquill.[2]

TABLE 1. KEY TO STABILITY CATEGORIES

SURFACE WIND SPEED (at 10m), m sec^{-1}	DAY			NIGHT	
	INCOMING SOLAR RADIATION			CLOUD	COVER
	STRONG	MODERATE	SLIGHT	>4/8	≤3/8
<2	A	A-B	B		
2-3	A-B	B	C	E	F
3-5	B	B-C	C	D	E
5-6	C	C-D	D	D	D
>6	C	D	D	D	D

Table 2 contains the required parameter values for flat, level and open terrain. Note that reference σ_y values, σ_{yr}, are given for both a continuous and an instantaneous source: continuous refers to emission times on the order of 10 minutes or more, while instantaneous represents emission times less than two and one-half seconds.

TABLE 2. RECOMMENDED VALUES OF PARAMETERS
(OPEN TERRAIN)
($x_{zr} = x_{yr} = 100$ meters)

Pasquill Stability Category	σ_{yr} (Contin) meters	σ_{yr} (Inst) meters	α	σ_{zr} meters	β	H_m meters
A	27.0	9.00	1.0	14.0	1.40	2750
B	19.0	6.33	1.0	11.0	1.00	2250
C	12.5	4.80	1.0	7.5	0.90	1750
D	8.0	4.00	0.9	4.5	0.85	875
E	6.0	3.00	0.8	3.5	0.80	125
F	4.0	2.00	0.7	2.5	0.75	30

Within wooded or forested areas, the Pasquill stability categories, and their associated meteorological parameter values, do not apply. Empirical data show that plumes under forest/jungle canopies tend to expand to much larger volumes, at shorter travel distances, than do those on flat, level and open terrain. Thus, the parameter values presented in Table 2 are not representative of forested environments. Empirical data also show that wind speeds under canopies are much lower than wind speeds external to the canopies at any given time. Thus, plumes travel much farther over flat, level and open terrain than they do in forests, under any given meteorological situation, in a given time. As a result, actual and predicted hazard distances could be markedly different for open versus forested terrains. Table 3 presents a set of meteorological parameter values for use in estimating hazard distances in forested environments. These empirically-based data were derived by members of the former US Army MUCOM Operations Research Group, from a variety of test data sources, only a few of which are referenced here.[6, 7, 8, 9]

TABLE 3. RECOMMENDED VALUES OF PARAMETERS
(FORESTED TERRAIN)
($x_{yr} = 100$ meters, $x_{zr} = 20$ meters)

REFERENCE WIND SPEED (mph) OUTSIDE CANOPY	TRANSPORT WIND SPEED, U (mph) UNDER CANOPY	σ_y	α	σ_z	β
Deciduous Forest, Winter					
1	0.2	12.8	0.80	1.3	1.20
5	1.0	12.1	1.00	1.4	1.20
12	2.4	12.0	1.00	1.5	1.20
20	4.0	12.0	1.10	1.5	1.20

TABLE 3. RECOMMENDED VALUES OF PARAMETERS, CONTINUED
(FORESTED TERRAIN)
(x_{yr} = 100 meters, x_{zr} = 20 meters)

REFERENCE WIND SPEED (mph) OUTSIDE CANOPY	TRANSPORT WIND SPEED, U (mph) UNDER CANOPY	σ_y	α	σ_z	β
Mixed Deciduous and Coniferous Forest, Winter					
1	0.2	18.2	0.80	1.6	1.30
5	0.8	17.5	1.00	1.7	1.30
12	1.8	16.8	1.00	1.7	1.30
20	3.0	14.5	1.00	1.7	1.30
Coniferous Forest					
1	0.2	23.5	0.80	1.8	1.30
5	0.8	22.5	1.00	1.9	1.30
12	1.8	19.0	1.00	1.9	1.30
20	3.0	14.0	1.00	1.9	1.30
Mixed Deciduous and Coniferous Forest, Summer and Deciduous Forest, Summer					
1	0.1	29.0	0.80	2.1	1.40
5	0.5	26.5	1.00	2.1	1.40
12	1.2	22.5	1.00	2.1	1.40
20	2.0	16.5	1.00	2.1	1.40
Tropical Rain Forest					
1	0.1	53.0	1.00	6.9	1.00
5	0.3	36.0	1.00	6.9	1.00
12	0.6	26.0	1.00	6.9	1.00
20	1.0	23.0	1.00	6.9	1.00

4.3. TOXICITY

Although the Basic Method can be used to estimate hazards from any airborne or spilled toxic substances, its principal application here is to hazards associated with operations involving chemical warfare agents. Required toxicity values are those which correspond to “1% lethalities” for lethal agents and “1% incapacitation” for incapacitating agents. Accordingly, appropriate toxicity values for a number of those agents are provided in Table 4.

TABLE 4. TOXICITY VALUES (mg-min/m^3)

CHEMICAL AGENT	1% INCAPACITATION	1% LETHALITIES
AC	N/A	1180
BZ	31	N/A
CG	N/A	385
CK	N/A	1850
DM	2240	N/A
GA	N/A	20
GB, GD, GF	N/A	10
H, HD, HN-1, HN-3	N/A	150
HT	N/A	75
L	150	N/A
VX (Inhalation)	N/A	4.3

Except as noted below, the entries in Table 4 are presented in terms of the total dosages (i.e., units are milligrams-minutes per cubic meter) required to produce 1% incapacitation (or 1% lethalities) among adults in a population where the average breathing rate is twenty-five liters per minute (i.e., moderate work activity). Those values can be reduced by one-third for children because of reduced body weights and greater air-intake-to-body-weight ratios.

Among the exceptions suggested above are the following:

a. The values presented for both CK and DM were developed from toxicity data related to “no deaths.” However, in the absence of better information, those values should be used for “1% lethalities” for CK and “1% incapacitation” for DM.

b. In the cases of H, HD, HN-1, HN-3 and L, there is no dependence on breathing rate for toxicological effects in the same sense that such relationships have been established for the other agents cited. The dosage of 150 mg-min/m^3 applies to no permanent skin injury. That value, in the absence of more definitive toxicological information on mustard, is used in lieu of the “1% lethality” dosage.

c. In the case of G and V agents, where the tabulated total dosages are reached as a result of exposure to small agent concentrations over extended time intervals (i.e., greater than two minutes), care must be taken to calculate hazards in accordance with the special methods described in Annex B.

d. VX toxicity values, shown in Table 4, are related only to inhaled vapor dosages. The “bare-skin” VX droplet deposit density corresponding to “1% lethalities” is 4.5 mg per man. That value increases rapidly as layers of clothing are added between the skin and the chemical agent droplets. As a result of any specific MCE, VX could pose a hazard through the deposition of droplets onto personnel as well as through the inhalation of vapors. In such cases, the contributions from both respiratory and percutaneous effects are calculated in terms of total agent (milligrams) within the body. The intravenous dose corresponding to “1% lethalities” is 0.1 mg.

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SUMMARY

A Gaussian Plume atmospheric diffusion model with (a) provisions for limiting the vertical expansion of a plume to the surface mixing layer and (b) criteria to accommodate the time-space variations of meteorological and other environmental factors has been recommended for application to hazard analyses. Two forms of the model, the Basic Model and a generalized model, have been recommended for applications where appropriate. The Basic Model can be used to compute the ground-level, axial, total dosage from accidents/incidents. Its use is adequate to treat the majority of hazard-distance estimation problems. One of many forms of the generalized model may be used to treat problems which involve (a) gravitational settling of particles or (b) computation of dosage and concentration at locations other than on plume centerlines, etc.

Input data and information adequate to permit application of both models to estimating hazard distances are provided. Among those data are meteorological parameter values, toxicity data for chemical warfare agents, methods for estimating evaporation rates of toxic substances from puddles, and methods for estimating the rate of rise of buoyant toxic plumes.

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ANNEX A

THE GENERALIZED PREDICITION MODEL

CONTENTS

ANNEX A

THE GENERALIZED PREDICTION MODEL

A.l. THE GENERALIZED MODEL CONCEPT

The concept of a generalized prediction model for use in CB applications was first outlined by Milly[1] who pointed out the necessity of finding a satisfactory technique for separating the effects of source factors and meteorological factors in assessing the performance of CB ammunition from field measurements. The generalized model concept has been broadened and implemented under various contracts sponsored by the U.S. Army Dugway Proving Ground and Deseret Test Center.[2, 3, 4, 5] The generalized prediction model, developed as a result of this work, is intended to be universally applicable to all chemical agent requirements including hazard-safety analyses. In principle, the generalized prediction model is adapted to these various requirements by substituting in the model sets of source factors and meteorological factors appropriate to the chemical ammunition and environmental regimes under consideration.

The formatting of the generalized prediction model begins with a simple mass continuity equation that in principle provides a complete description of the dilution and depletion of a cloud of airborne material as it is transported downwind from the point of formation to all travel distances of interest. The generalized concentration model format, for example, must explicitly specify:

1. The downwind trajectory and the rate at which the cloud moves along this trajectory.

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[1] Milly, G. H., "Atmospheric Diffusion and Generalized Munitions Expenditure (U)", ORG Study No. 17, US Army Chemical Corps Operations Research Group, Army Chemical Center, MD, 1 May 1958. UNCLASSIFIED.

[2] Cramer, H. E., et al, "Meteorological Prediction Techniques and Data Systems", GCA Tech Report No. 64-3-G, Final Report under Contract DA-42-007-CML-552, US Army Dugway Proving Ground, Dugway, UT, 1964.

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[5] Cramer, H. E. and R. K. Dumbauld, "Experimental Designs for Dosage Prediction in CB Field. Tests", GCA Tech Report No. 68-17-G, Final Report under Contract DA-42-007-AMC-276(R), US Army Dugway Proving Ground, Dugway, UT, 1968.

2. The lateral, vertical and alongwind dimensions of the cloud as functions of downwind-distance or travel time.

3. The form of the distribution of material along each of the three coordinate axes.

4. Losses of material by simple decay processes, precipitation scavenging, gravitational settling and other removal processes.

5. Variations in initial cloud dimensions, source-emission time, meteorological structure, terrain, and vegetative cover.

In generic form, the generalized concentration model is conveniently expressed by the product of five terms:

$$\text{Concentration} = \left(\text{Peak Concentration Term}\right) \cdot\cdot \left(\text{Alongwind Term}\right) \cdot \\ \left(\text{Lateral Term}\right) \cdot\cdot \left(\text{Vertical Term}\right) \cdot\cdot \left(\text{Depletion Term}\right)$$

where the Peak Concentration Term refers to the concentration at the centroid of the cloud; the Depletion Term refers to the loss of material by the various processes mentioned above; and the remaining three terms define the dimensions of the cloud with respect to a conventional Cartesian coordinate system. As long as mass continuity is satisfied, there are no restrictions on the expressions that may be substituted for the various terms in the generalized model equation or on the form of the coordinate system. Thus, almost any diffusion model may be substituted in the generalized model equation. The generalized dosage model contains only four terms and has the same format as the generalized concentration model, except for the elimination of the Alongwind Term and the substitution of a Peak Dosage Term for the Peak Concentration Term.

Application of the generalized model requires meteorological input parameters that are representative of the atmospheric structure within a reference three-dimensional-air volume that extends downwind from the source to maximum cloud travel distance of interest. The reference volume may contain from one to several hundred cubic miles of air. The maximum height of the reference volume is usually given by the depth of the surface mixing layer H_m. The bulk of the meteorological parameters required as direct inputs to the generalized models are obtained from space-time averaged vertical profiles of:

1. Turbulent intensities of the orthogonal wind-velocity components.

2. Mean wind speed.

3. Mean azimuth wind direction.

4. Air temperature.

representative of the reference air volume. Other meteorological parameters required by the model include rainout and washout coefficients as well as information on the intensity, areal extent and duration of precipitation. The effects of terrain and other surface properties are principally taken into account in the generalized model by changing the meteorological inputs to conform to particular combinations of atmospheric stability and surface roughness elements. The development of internally consistent sets of meteorological parameters that are representative of specific environmental regimes is one of the primary prerequisites for the successful application of quantitative concentration-dosage prediction methods to chemical agent problems. This is an important point because the inherent interdependence of the meteorological model inputs precludes arbitrary variations in individual parameters while holding all other parameters fixed.

It is important to recognize that the generalized concentration and dosage models described below are inherently interim models and that specific provision should be made for updating them as new information becomes available. In many instances, the appropriate source and meteorological input information is almost completely lacking and can only be acquired empirically. Also, model validation is basically a long-term process because of similar inadequacies in existing concentration, dosage, and meteorological measurements.

The model equations presented below contain Gaussian distribution functions and are based on a conventional Cartesian coordinate system with the origin placed at ground level directly below the source. The auxiliary equations for lateral and vertical cloud expansions are expressed in terms of simple power laws in which the standard deviations of wind azimuth and elevation angle are used as prime predictors. It should be noted that, for many chemical agent applications, mesoscale factors control the diffusion and depletion processes. The factors that are most important in determining the concentrations and dosages at distances greater than a few kilometers downwind from the point of release are the depth of the surface mixing layer, the vertical shear of wind speed, and azimuth wind direction in the surface mixing layer. It follows that, at these distances, the choice of expressions used in the models to account for microscale turbulent expansion is frequently not of critical importance.

A.2. GENERALIZED CONCENTRATION MODEL FOR POINT OR VOLUME SOURCES

A.2.1. Generalized Concentration Model

The generalized concentration model for instantaneous point or volume sources is expressed as the product of five terms:

$$\text{Concentration} = \left(\text{Peak Concentration Term}\right) \cdot \left(\text{Alongwind Term}\right) \cdot \left(\text{Lateral Term}\right) \cdot \left(\text{Vertical Term}\right) \cdot \left(\text{Depletion Term}\right) \qquad \text{(A.1)}$$

The Peak Concentration Term is defined by the expression

$$\frac{KQ}{(2\pi)^{3/2}\,\sigma_z\sigma_y\sigma_x} \qquad (A.2)$$

where

Q = source strength

K = scaling coefficient used to convert input parameters into dimensionally consistent units

σ_z = standard deviation of the vertical concentration distribution

σ_y = standard deviation of the crosswind concentration distribution

σ_x= standard deviation of the alongwind concentration distribution

The Vertical Term refers to the expansion of the cloud in the vertical or z direction and includes terms for limiting the vertical cloud growth to the depth of the surface mixing layer.

$$\text{Vertical Term} = \left\{ \exp\left[-\frac{1}{2}\left(\frac{H-z}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{H+z}{\sigma_z}\right)^2\right] + \sum_{i=1}^{\infty}\left[\exp\left[-\frac{1}{2}\left(\frac{2iH_m-H-z}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{2iH_m-H+z}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{2iH_m+H-z}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{2iH_m+H+z}{\sigma_z}\right)^2\right]\right]\right\} \qquad (A.3)$$

where

H = effective source height

H_m = depth of the surface mixing layer

z = height abovc ground

The Lateral Term refers to the crosswind expansion of the cloud and includes reflection terms for limiting lateral cloud growth in the presence of topographical barriers.

$$\text{Lateral Term} = \Bigg\{ \exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right] + \sum_{i=1}^{\infty}\Bigg[\exp\left[-\frac{1}{2}\left(\frac{2i\left(y_1+y_2\right)-y}{\sigma_y}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{2i\left(y_1+y_2\right)+y}{\sigma_y}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{2i\left(y_1+y_2\right)-2y_2-y}{\sigma_y}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{2i\left(y_1+y_2\right)-2y_1+y}{\sigma_y}\right)^2\right]\Bigg]\Bigg\} \quad \text{(A.4)}$$

where

y = lateral distance from cloud centerline

y_1 = lateral distance from the source to the reflecting surface on the right of the source looking downwind

y_2 = lateral distance from the source to the reflecting surface on the left of the source looking downwind

The Alongwind Term refers to cloud growth in the downwind or x direction

$$\text{Alongwind Term} = \exp\left[-\frac{1}{2}\left(\frac{x-\tilde{u}t}{\sigma_x}\right)^2\right] \quad \text{(A.5)}$$

where

$\tilde{u}$ = mean cloud transport speed over the distance interval from the point of cloud stabilization to the downwind distance x

t = time after cloud stabilization

The Depletion Term refers to the loss of material by simple decay processes, precipitation scavenging, or gravitational settling. The form of the Depletion Term for each of these processes is:

$$\text{(Decay)} \quad \exp\left[-k\bar{t}\right] \quad \text{(A.6)}$$

$$\text{(Precipitation Scavenging)} \quad \exp\left[-\Lambda\left(\frac{x}{\tilde{u}}-t_1\right)\right] \quad \text{(A.7)}$$

$$\text{(Gravitational Settling)} \quad \left\{ \exp\left[-\frac{1}{2}\left(\frac{H-\left(V_s\, x/\bar{u}_H\right)-z}{\sigma_z}\right)^2\right] + \exp\left[-\frac{1}{2}\left(\frac{2H_m-H+\left(V_s\, x/\bar{u}_H\right)-z}{\sigma_z}\right)^2\right]\right\} \tag{A.8}$$

Where

k = decay coefficient or fraction of material lost per unit time

$\bar{t}$ = mean cloud travel time = $x/\bar{u}$

Λ = washout coefficient or fraction of material removed by scavenging per unit time

V_s = gravitational settling velocity for a given particle size

$\bar{u}_H$ = mean wind speed between the ground and H

t_1 = time rain begins

When Equation (A.8) is used for the Depletion Term, the Vertical Term given by Equation (A.3) is set equal to unity. Equation (A.8) causes the cloud axis to be inclined downwind at the angle $\tan^{-1}(V_s/\bar{u}_H)$ with respect to the horizon, following W. Schmidt's sedimentation hypothesis.[2] Material which deposits on the ground is retained and not reflected. The vertical growth of the cloud is stopped at the top of the surface mixing layer and reflected toward the ground by the second exponential term in Equation (A.8). The depletion by gravitational settling of material containing a size distribution is calculated by partitioning the distribution into settling-velocity categories, solving Equation (A.1) for each settling velocity, and superposing the solutions.

The peak concentration χ_p at distance x and at an arbitrary distance $y \neq 0$ from the cloud center line is given by

$$\chi_p\{x,y,z,t=x/\bar{u}\} = \chi/\ \{\text{Alongwind Term}\} \tag{A.9}$$

Similarly, the peak concentration χ_{mp} at distance x on the cloud centerline $y = 0$ is given by the expression

$$\chi_{mp}\ \{x,y=0,z,t=x/\bar{u}\} = \chi/\{\text{Alongwind Term}\}\ \{\text{Lateral Term}\} \tag{A.10}$$

A.2.2. Subset of Equations for σ_z, σ_y, and σ_x

The subset of equations defining the distance dependence of the standard deviations of the vertical, crosswind and alongwind concentration distributions in given below.

The standard deviation of the vertical concentration distribution is given by the expression

$$\sigma_z = \sigma'_E \, x_{zr} \left[\frac{x + x_z - x_{zr}(1-\beta)}{\beta \, x_{zr}} \right]^{\beta} \qquad \text{(A.11)}$$

where

σ'_E = standard deviation of the elevation wind angle in radians at height H

x_{zr} = distance over which rectilinear vertical cloud expansion occurs downwind from an ideal point source

β = vertical diffusion coefficient

x_z = vertical virtual distance

$$= \begin{cases} \dfrac{\sigma_{zR}}{\sigma'_E} - x_{zR} & ; \; \sigma_{zR} \leq \sigma'_E x_{zr} \\[2ex] \beta \, x_{zr} \left(\dfrac{\sigma_{zR}}{\sigma'_E \, x_{zr}} \right)^{1/\beta} - x_{zR} + x_{zr}(1-\beta) & ; \; \sigma_{zR} > \sigma'_E x_{zr} \end{cases} \qquad \text{(A.12)}$$

σ_{zR} = standard deviation of the vertical concentration distribution at a distance x_{zR} downwind from the source.

The standard deviation of the crosswind concentration distribution is given by the expression

$$\sigma_y = \left[\left(\sigma'_A\{\tau\} \, x_{yr} \left(\frac{x + x_y - x_{yr}(1-\alpha)}{\alpha \, x_{yr}} \right)^{\alpha} \right)^2 + \left(\frac{\Delta \theta' \, x}{4.3} \right)^2 \right]^{1/2} \qquad \text{(A.13)}$$

where

σ'_A = standard deviation of the azimuth wind angle in radians at height H measured over the source emission time τ

$$= \sigma'_A\{\tau_o\} \left(\frac{\tau}{\tau_o} \right)^{1/5} \qquad \text{(A.14)}$$

$\sigma'_A\{\tau_o\}$ = standard deviation of the aximuth wind angle in radians in the surface mixing layer measured over the reference time τ_o

x_{ry} = distance over which rectilinear crosswind cloud expansion occurs downwind from the virtual point source

α = crosswind diffusion coefficient

x_y = crosswind virtual distance

$$= \left\{ \begin{array}{ll} \dfrac{\sigma_{yR}}{\sigma'_A\{\tau\}} - x_{yR} & ; \ \sigma_{yR} \leq \sigma'_A\{\tau\} x_{yr} \\ \alpha x_{yr} \left(\dfrac{\sigma_{yR}}{\sigma'_A\{\tau\} x_{yr}} \right)^{1/\alpha} - x_{yR} + x_{yr}(1-\alpha) & ; \ \sigma_{yR} > \sigma'_A\{\tau\} x_{yr} \end{array} \right\} \quad (A.15)$$

σ_{yR} = standard deviation of the crosswind concentration distribution at a distance x_{Ry} downwind from the source

$\Delta\theta'$ = azimuth wind direction shear in radians within the layer containing the cloud

$$= \frac{\Delta\theta}{\Delta z} \cdot \frac{\pi}{180} \left(z_2 - z_1 \right)$$

$\frac{\Delta\theta}{\Delta z}$ = rate change of wind direction in degrees with height in the surface mixing layer where $\Delta\theta$ is positive in the clockwise sense

z_2 = effective upper bound of cloud

z_1 = effective lower bound of cloud

The standard deviation of the alongwind concentration distribution is given by the expression

$$\sigma_x = \left\{ \left(\frac{L\ (x)}{4.3} \right)^2 + \sigma_{xo}^{\ 2} \right\}^{1/2} \qquad (A.17)$$

where

L (x) = alongwind cloud length at distance x from the source

$$= \left\{ \begin{array}{lll} \dfrac{E\ (\Delta\tilde{u})x}{u} & ; & \Delta\bar{u} \geq 0 \\ 0 & ; & \Delta\bar{u} < 0 \end{array} \right\} \qquad (A.18)$$

Δu = vertical wind speed shear in the layer containing the cloud

σ_{xo} = standard deviation of the alongwind concentration distribution at the source

E = the efficiency factor for alongwind growth due to vertical wind speed shear

The expression for L (x) given by Equation (A.18) is based on the work of Tyldesley and Wallington.[6] This expression assumes that the alongwind growth produced by wind speed shear is normally much larger than the alongwind growth produced by turbulence alone. On the basis of theory and limited field data, Tyldesley and Wallington assign a mean value to E of 0.28. However, more recent measurements made in the United States and Canada suggest that E set equal to 0.6 to 0.7 more accurately describes alongwind cloud growth.

An alternate, simpler expression for the standard deviation of the alongwind concentration was developed by Halvey[7] from a study of observed values obtained from long distance cloud travel. These data included the observations used by Tyldesley and Wallington[6] and other observations collected for greater distances.

Halvey's equation is:

$$\sigma_x = .1522\left(x\right)^{.9294} \qquad \text{(A.18a)}$$

A.2.3 Subset of Equations for u and $\bar{u}_H$

The mean cloud transport speed at a downwind travel distance x is defined by the expression

$$\bar{u}(x) = \frac{1}{(z_2 - z_1)} \int_{z_1}^{z_2} \bar{u}(z)\, dz \qquad \text{(A.19)}$$

If the vertical profile of mean wind speed is given by a simple power law.

$$\bar{u}(z) = \bar{u}_R\left(\frac{z}{z_R}\right)^p$$

Equation (A.19) can be integrated to yield

$$\bar{u}(x) = \frac{\bar{u}_R\left[(z_2)^{1+p} - (z_1)^{1+p}\right]}{(z_2 - z_1)\ (z_R)^p\ (1+p)} \qquad \text{(A.20)}$$

where

$\bar{u}_R$ = mean wind speed at the reference height z_R

p = wind power-law exponent

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[6] Tyldesley J. and Wallington W., The Effect of Wind Shear and Vertical Diffusicn on Horizontal Dispersion, Quarterly Journal of the Roya1 Meteorological Society, Volume 91: Pages 158-174, 1965.

[7] Halvey, David D., Estimation of Cloud Length for Long Distance Travel, Unpublished Report, Operations Research Group, Edgewood Arsenal, MD, July 1973.

The integration limits z_1 and z_2 correspond to the effective lower and upper bounds, respectively, of the layer containing the cloud and may be expressed in terms of the height of the cloud centerline H and the standard deviation of the vertical concentration or dosage distribution as:

$$z_1 = \left\{ \begin{array}{lll} H - 2.15\,\sigma_z & ; & H - 2.15\,\sigma_z > 0 \\ 0 & ; & H - 2.15\,\sigma_z \leq 0 \end{array} \right\} \qquad \text{(A.21)}$$

$$z_2 = \left\{ \begin{array}{lll} H + 2.15\,\sigma_z & ; & H + 2.15\,\sigma_z \leq H_m \\ H_m & ; & H + 2.15\,\sigma_z > H_m \end{array} \right\} \qquad \text{(A.22)}$$

The mean cloud transport speeds over the distance interval from the point of stabilization to the downwind distance x is then given by

$$\tilde{u} = \frac{1}{x} \int_0^x \tilde{u}\,\{x\}\,dx \qquad \text{(A.23)}$$

This wind speed is calculated numerically in computer programs by summing values of $\bar{u}\{x\}$ calculated at 10-meter intervals from the source to distance x and dividing by the number of intervals. Similarly, the mean wind speed shear $\Delta\bar{u}$ is numerically calculated from the expression

where

$$\Delta\tilde{u} = \frac{1}{x} \int_0^x \Delta\bar{u}\,\{x\}\,dx \qquad \text{(A.24)}$$

$$\Delta\bar{u}\,\{x\} = \frac{\bar{u}_R}{z_R^{\,p}} \left(z_2^{\,p} - z_1^{\,p} \right) \qquad \text{(A.25)}$$

The mean wind speed $\bar{u}_H$ between the ground and effective source height H is defined by the expression

$$\bar{u}_H = \left\{ \begin{array}{lll} \dfrac{\bar{u}_R \left[(H)^{1+p} - \left(z_R\right)^{1+p} \right]}{\left(z_R\right)^p \left(H - z_R\right) \left(1+p\right)} & ; & H > z_R \\ \bar{u}_R & ; & H \leq z_R \end{array} \right\} \qquad \text{(A.26)}$$

A.2.4. Generalized Dosage Model

The generalized dosage mode for point and volume sources is given by the product of four terms:

$$\text{Dosage} = \{\text{Peak Dosage Term}\}\ \{\text{Vertical Term}\}\ \{\text{Lateral Term}\}\ \{\text{Depletion Term}\} \tag{A.27}$$

Except for the Peak Dosage Term, the terms in the dosage equation correspond to the same terms defined in the preceding section for the concentration model. Also, the subsets of equations for σ_y, σ_z, and $\bar{u}$ given in the preceding section apply to the dosage model.

The Peak Dosage Term refers to the dosage on the downwind axis of the cloud (x, y=O, z=H) and is defined by the expression

$$\frac{K\,Q}{2\pi\ \bar{u}\{x\}\ \sigma_y\ \sigma_z} \tag{A.28}$$

where

Q 2 = source strength

K = scaling coefficient used to convert input parameters into dimensionally consistent Units

σ_y = standard deviation of the crosswind dosage distribution

σ_z = standard deviation of the vertical dosage distribution

A.3. APPLICATION OF THE GENERALIZED MODEL TO CONCENTRATIONS PRODUCED BY QUASI-CONTINUOUS RELEASES

The concentrations produced by a quasi-continuous release in which the emission takes place over a period of several minutes to several hours may be obtained by multiplying Equation (A.27) by an Alongwind Term. For a release with a constant rate Q for a finite period r, the Alongwind Term is given by

$$\{\text{Alongwind Term}\} = \frac{1}{2}\left[\operatorname{erf}\left(\frac{x-\tilde{u}(t-\tau)}{\sqrt{2}\,\sigma_x}\right) - \operatorname{erf}\left(\frac{x-\tilde{u}\,t}{\sqrt{2}\,\sigma_x}\right)\right] \tag{A.29}$$

Note that the emission rate Q rather than the total source strength Q must be used in calculating concentrations for this type of release.

In the case of an evaporative spill, the emission rate can be expected to decay exponentially with time. For this type of release, the Alongwind Term is given by

$$\{\text{Alongwind Term}\} = \frac{\lambda}{2}\left\{\exp\left[-\frac{1}{2}\left(\frac{\sigma_x^2\,\lambda^2}{\tilde{u}^2} + \frac{2\lambda(x-\tilde{u}t)}{\tilde{u}}\right)\right]\right\}$$

$$\left\{\operatorname{erf}\left[\frac{x-\tilde{u}(t-\tau)}{\sqrt{2}\,\sigma_x} + \frac{\sigma_x\,\lambda}{\sqrt{2}\,\tilde{u}}\right] - \operatorname{erf}\left[\frac{(x-\tilde{u}t)}{\sqrt{2}\,\sigma_x} + \frac{\sigma_x\,\lambda}{\sqrt{2}\,\tilde{u}}\right]\right\} \tag{A.30}$$

where λ, is the evaporation coefficient, or the fraction of material evaporated per unit time. For this type of release, the total source strength Q is entered in Equation (A.27). Additionally, the initial alongwind dimension σ_{xo} is set equal to zero in the σ_x calculations.

A.4. APPLICATION OF THE GENERALIZED MODEL TO SURFACE DEPOSITIOH BY GRAVITATIONAL SETTLING

Equation (A.27) may also be used to calculate the surface deposition due to gravitational settling by replacing the Vertical Tern in Equation (A. 27) with the following expression:

$$\{\text{Vertical Term}\} = \tilde{u}\{x\}\left\{\left[\frac{\beta H + \left(\left(1-\left(\frac{\beta x}{x+x_z-x_{zr}(1-\beta)}\right)\right)V_s\left(x+x_z-x_{zr}(1-\beta)\right)/\tilde{u}_H\right)}{\left(x+x_z-x_{zr}(1-\beta)\right)}\right]\right.$$

$$\cdot \exp\left[-\frac{1}{2}\left(\frac{H-\left(V_s x/\tilde{u}_H\right)}{\sigma_z}\right)^2\right]$$

$$+\left[\frac{\beta\left(2H_m-H\right)-\left(\left(1-\left(\frac{\beta x}{x+x_z-x_{zr}(1-\beta)}\right)\right)V_s\left(x+x_z-x_{zr}(1-\beta)\right)/\tilde{u}_H\right)}{\left(x+x_z-x_{zr}(1-\beta)\right)}\right]$$

$$\left.\cdot \exp\left[-\frac{1}{2}\left(\frac{2H_m-H+\left(V_s x/\tilde{u}_H\right)}{\sigma_z}\right)^2\right]\right\} \tag{A.31}$$

A.5. ADJUSTMENTS OF THE GENERALIZED MODEL FOR CXANGES XN METEOROLOGICAL STRUCTURE: THE STABILILTY-CHANGE MODEL

The generalized prediction model formulas, given above, assume steady-state conditions throughout the reference air volume which may extend vertically for 3 kilometers and downwind for 100 kilometers or more. In many instances, the steady-state assumption fails because of changes in surface properties and atmospheric structure that occur along downwind cloud trajectories. Techniques have been developed for adjusting the models to these changes which treat the changes as step-changes in meteorological structure. At any specified travel time or downwind-distance at which a step change in structure occurs, the transport and diffusion processes are stopped; new sets of source and meteorological model inputs are calculated; and the transport and diffusion process restarted with the new inputs. Thus, the procedures account for the effects of step-changes in atmospheric stability on the concentration, dosage, and deposition patterns in a gradual manner.

When the calculated generalized model distance exceeds the maximum downwind distance (This maximum downwind distance is calculated by the product of the mean transport speed and the maximum in-time duration for the stable regime.) that could exist in stable conditions, the stability change-model is used. The maximum time duration of a stable nighttime regime is generally 12 hours or less. Mean cloud transport speeds for stable regimes approximate 1 meter per second (2.24 miles per hour) with a maxim distance of approximately 40 kilometers (25 miles). Whenever the calculated hazard distance exceeds the cloud-transport distance under stable conditions, the stability-change model is used.

In the stability-change model, the mixing depth may be continuously varied by using the following Vertical Term in the generalized models:

$$\{\text{Vertical Term}\} = \frac{\sqrt{2\pi}\,\sigma_z}{H_m\{x\}}$$

where

$$H_m\{x\} = \left\{ H_{m_i} + \left[\frac{H_{m_{i+1}} - H_{m_i}}{x_{i+1} - x_i} \right] \left(x - x_i \right) \; ; \quad x > x_i \right\} \qquad \text{(A.33)}$$

H_{m_i} = median mixing depth for the i^{th} stability category

x_i = downwind distance from the point of cloud stabilization to the cloud center at the time that the i^{th} stability category ends

The only restriction to the use of the above Vertical Term is that the cloud must fill the mixing layer and be completely mixed in the vertical (i.e., the concentration must be uniform with height).

ANNEX B

TOXICITY FOR GB AND VX AS A FUNCTION OF EXPOSURE TIME

CONTENTS

LIST OF FIGURES

ANNEX B

TOXICITY FVR GB AND VX AS A FUNCTION OF EXPOSURE TIME

B.1. GENERAL. This methodology is required to implement the changes in effective dosages of GB and VX as a function of exposure time in agent clouds of nonuniform concentration. Dosage, usually denoted D or Ct , is defined as the product of agent concentration at a point and the time of exposure to those agent concentrations. Thus, exposure time for a given Ct is a factor which influences the relationships between dosage and expected physiological response. Increasing the exposure time to a given Ct results in a less severe toxic response. To produce the same toxic response, higher Ct exposures are required for long exposure times than for short ones. As an example, an estimated LCt_{50} value for a man breathing 10 l/min is 100 mg-min/m^3 for a two minute exposure, while the LCt_{50} value is estimated as 210 mg-min/m^3 for a 30-minute exposure. The relationship between exposure time and LCt_{50} is shown in Figure B.1.[1] Because the effective Ct exposure is dependent on the time, the degree of hazard will be reduced in those accidents where the vapor is evolved slowly over a substantial time as compared with nearly instantaneous releases such as would occur in detonation of a GB munition.

B.2. THE BASIC MODEL. The basic model for calculating peak dosage at ground level (y = 0, zero) as a function of distance and time may be expressed as

$$D(x, \Delta\theta) = \frac{Q}{\pi \sigma_y \sigma_z U_x} \cdot \left\{ \exp - \frac{1}{2}\left(\frac{H}{\sigma_z}\right)^2 + \sum_{i=1}^{\infty} \left[\exp - \frac{1}{2}\left(\frac{2iH_m + H}{\sigma_z}\right)^2 + \exp - \frac{1}{2}\left(\frac{2iH_m - H}{\sigma_z}\right)^2 \right] \right\} \cdot \frac{1}{2}\left\{ \operatorname{erf}\left(\frac{x - U_x\theta_1}{\sqrt{2}\,\sigma_x}\right) - \operatorname{erf}\left(\frac{x - U_x\theta_2}{\sqrt{2}\,\sigma_x}\right) \right\} \qquad (B.1)$$

where $\theta_{1,2}$ = time subsequent to agent dissemination ($\theta_2 > \theta_1$)

$\Delta\theta = \theta_2 - \theta_1$

where

$\theta_{1,2}$ = time subsequent to agent dissemination ($\theta_2 > \theta_1$)

$\Delta\theta = \theta_2 - \theta_1$

---

[1] Christensen, M. K., P. Cresthull, and F. W. Oberst. Chemical Warfare Laboratories Report No. 2266, ICt_{1-99} and LCt_{1-99} Estimates of GB Vapor for Man at Various Exposure Times, US Army Chemical Warfare Laboratories, Army Chemical Center, MD. December 1958. UNCLASSIFIED.

$$\sigma_y(x) = \sigma_{yr}\left(\frac{x}{x_{yr}}\right)^{\alpha}$$

$$\sigma_z(x) = \sigma_{zr}\left(\frac{x}{x_{zr}}\right)^{\beta}$$

$$\sigma_x(x) = .1522\ (x)^{.9294}$$

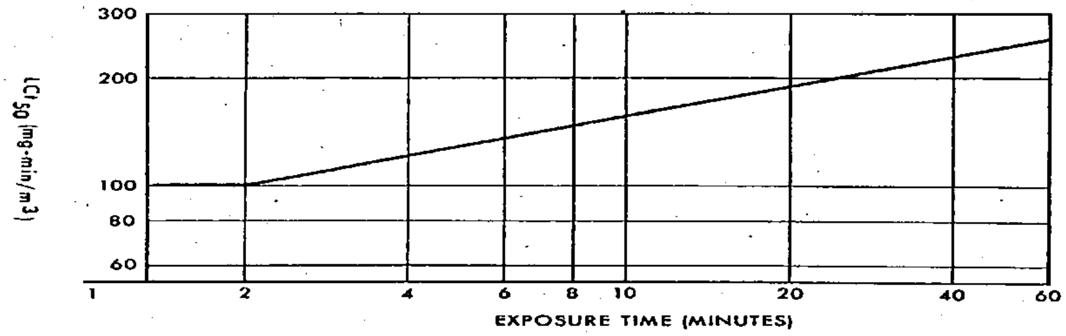

Figure B.1: Change of LCt_{50} with Exposure Time in Men Breathing 10 ℓ/min and Exposed to GB Vapor

B.3. DOSAGE BUILDUP

For an instantaneous source, dosage buildup at a point as a function of time is readily determined from Equation (B.1). For agent generated at a uniform rate, dQ/dt, for a time period from the initiation of emission ($\theta_0 = 0$) to θ_S, computation of the dosage for an arbitrary interval $\Delta\theta = \theta_2 - \theta_1$ requires application of the more complicated expressions:

$$D(x,y,z;\Delta\theta) = \left\{\begin{matrix} K(T_5 - T_2 + T_4) & \text{for } \theta_s \geq \theta_2 > \theta_1 \\ K(T_1 - T_2 - T_3 + T_4) & \text{for } \theta_2 > \theta_1 \geq \theta_s \end{matrix}\right\}$$

where

$$K = \frac{dQ/dt}{2\pi\sigma_y\sigma_z U}\cdot$$

$$\left\{\exp -\frac{1}{2}\left(\frac{H}{\sigma_z}\right)^2 + \sum_{i=1}^{\infty}\left[\exp -\frac{1}{2}\left(\frac{2iH_m+H}{\sigma_z}\right)^2 + \exp -\frac{1}{2}\left(\frac{2iH_m-H}{\sigma_z}\right)^2\right]\right\},$$

$$T_1 = (\theta_2-\theta_s-\frac{x}{u_x})\ \text{erf}\left\{\frac{x-u_x(\theta_2-\theta_s)}{\sqrt{2}\ \sigma_x}\right\} - (\theta_1-\theta_s-\frac{x}{u_x})\ \text{erf}\left\{\frac{x-u_x(\theta_1-\theta_2)}{\sqrt{2}\cdot\sigma_x}\right\}$$

$$T_2 = (\theta_2 - \frac{x}{u_x})\ \text{erf}\left\{\frac{x-u_x\theta_2}{\sqrt{2}\ \sigma_x}\right\} - (\theta_1 - \frac{x}{u_x})\ \text{erf}\left\{\frac{x-u_x\theta_1}{\sqrt{2}\ \sigma_x}\right\} \quad (B.2)$$

$$T_3 = \frac{\sqrt{2}\,\sigma_x}{\sqrt{\pi}\,u_x}\left[\exp\left\{-\frac{[x-u_x(\theta_2-\theta_s)]^2}{2\,\sigma_x^2}\right\} - \exp\left\{-\frac{[x-u_x(\theta_1-\theta_s)]^2}{2\,\sigma_x^2}\right\}\right]$$

$$T_4 = \frac{\sqrt{2}\,\sigma_x}{\sqrt{\pi}\,u_x}\left[\exp\left\{-\frac{(x-u_x\theta_2)^2}{2\,\sigma_x^2}\right\} - \exp\left\{-\frac{(x-u_x\theta_1)^2}{2\,\sigma_x^2}\right\}\right]$$

$$T_5 = (\theta_2 - \theta_1)\,\mathrm{erf}\left\{\frac{x}{\sqrt{2}\,\sigma_x}\right\} \qquad \text{(B.3)}$$

If $\theta_1 < \theta_s < \theta_2$, the total time period is partitioned into the segments θ_1 to θ_s and θ_s to θ_2. The dosage contribution for each time segment is derived separately from the appropriate form of the equation and the results added. Equation (B.1) is also readily adapted to cases of variable rate of agent generation, provided the total emission time can be divided into a set of intervals for each where a constant $\dot{Q}$ can be assumed. The contribution of a "source segment," as defined by $\dot{Q}$ over a given time interval, to the total dosage accumulated during $\Delta\theta$ may be computed independently for each such segment from Equation (B.1)*. The sum over the set of values so obtained is the total dosage of interest.

It follows from the accompanying figure that an effective dosage for an exposure time t (expressed in minutes) can be obtained by multiplying the corresponding reference "two-minute" value by the factor

$$M = 0.827\,t^{0.274} \qquad (t \geq 2 \text{ minutes}) \qquad \text{(B.4)}$$

A rationale was developed for the computation of the multiplier M by means of a numerical procedure that allows for discrete changes in agent concentration as the cloud moves over a ground location. In essence, a "pseudo" exposure time is determined through a sequence of adjustments for successive time increments covering cloud passage. This "pseudo" exposure time, which must be two minutes or greater for Equation (B.2) to be applicable, can be considered essentially as an integrated average. The precise sequential mathematical procedure is as follows:

Let t_i = clock time in minutes

T_i = "pseudo" exposure time in minutes

ΔD_i = dosage accumulation in interval i

D_i = cumulative dosage to time t_i

D_{oi} = two-minute reference dosage

---

*In applying Equation (B.1) it should be noted that agent emission is defined in the expressions as occurring from the origin (θ_0=0) of the time scale to θ_s. For cases involving a series of uniform generation rates, appropriate translations of the time scale (i,e., agent emission from θ_a to θ_b) will be necessary.

Subscript m denotes value computed from transport and diffusion model.
Subscript e denotes extrapolated value as indicated below.

1st Interval: Select clock time interval $t_0 \rightarrow t_1$: $(t_1 - t_0) \geq 2$ min

a. Determine D_{1m} for interval $t_1 - t_0$ from transport and diffusion model.

b. Set $\tau_1 = t_1 - t_0$.

c. Compute

$$D_{01} = \frac{D_{1m}}{(0.827)(\tau_1)^{0.274}}$$

2nd Interval: Select clock time interval $t_1 \rightarrow t_2$

a. Determine ΔD_{2m} for interval t_2-t_1 from transport and diffusion model.

b. Compute (1) $D_{2m} = D_{1m} + \Delta D_{2m}$

(2) $D_{2e} = 0.827\ D_{01}\ \ (\tau_1 + t_2 - t_1)^{0.274} - (t_1)^{0.274}$

c. Compare ΔD_{2m} with ΔD_{2e}

(1) If $\Delta D_{2m} = \Delta D_{2e}$, set $\tau_2 = \tau_1 + t_2 - t_1$

(2) If $\Delta D_{2m} > \Delta D_{2e}$, compute

(a) $D_{2e} = D_{1m} + \Delta D_{2e}$

(b) $$\tau_2 = \left[\frac{D_{2e}(\tau_1 + t_2 - t_1)^{0.274} + (\Delta D_{2m} - \Delta D_{2e})\ (t_2 - t_1)^{0.274}}{D_{2m}} \right]^{\frac{1}{0.274}}$$

(3) If $\Delta D_{2m} < \Delta D_{2e}$, compute

$$\tau_2 = \left[\frac{\frac{\Delta D_{2m}}{t_2 - t_1}\ (t_2 - t_0)(\tau_1 + t_2 - t1)^{0.274} + \left\{ D_{1m} - \frac{\Delta D_m}{t_2 - t_1}\ \ (t_1 - t_0) \right\} \tau_1{}^{0.274}}{D_{2m}} \right]^{\frac{1}{0.274}}$$

d. Compute $D_{02} = \dfrac{D_{2m}}{0.827(\tau_2)^{0.274}}$

General Case: Select clock time interval $t_{i-1} \rightarrow t_i$

a. Determine ΔD_{im} for interval t_i-t_{i-1} from transport and diffusion model.

b. Compute:

(1) $D_{im} = D_{(i-l)m} + \Delta D_{im}$

$$(2)\quad \Delta D_{ie} = 0.827\, D_{0(i-1)} \left[(\tau_{i-1}+t_i-t_{i-1})^{0.274} - (\tau_{i-1})^{0.274} \right]$$

c. Compare ΔD_{im} with ΔD_{ie}:

(1) If $\Delta D_{im} = \Delta D_{ie}$, set $\tau_i = \tau_{i-1} + t_i - t_{i-1}$

(2) If $\Delta D_{im} > \Delta D_{ie}$, compute

(a) $D_{ie} = D_{(i-1)m} + \Delta D_{ie}$

(b) $$\tau_i = \left[\frac{D_{ie}(\tau_{i-1}+t_i-t_{i-1})^{0.274} + (\Delta D_{im}-\Delta D_{ie})(t_i-t_{i-1})^{0.274}}{D_{im}} \right]^{\frac{1}{0.274}}$$

(3) If $\Delta D_{im} < \Delta D_{ie}$, compute

$$\tau_i = \left[\frac{\frac{\Delta D_{im}}{t_i-t_{i-1}}(t_i-t_0)(\tau_{i-1}+t_i-t_{i-1})^{0.274} + \left\{ D_{(i-1)m} - \frac{\Delta D_{im}}{t_i-t_{i-1}}(t_{i-1}-t_0) \right\} \tau_{i-1}^{0.274}}{D_{im}} \right]^{\frac{1}{0.2}}$$

d. Compute $D_{0i} = \dfrac{D_{im}}{0.827(\tau_i)^{0.274}}$

For n increments, the reference two-minute dosage D_{On} is the value used in constructing the generalized curves for GB and VX respiratory effects.

In using the above procedure, three precautions must be observed. Firstly, τ_i cannot be permitted to decrease below two minutes. Although such occurrence would generally be unlikely, the possibility should be recognized in the computational procedure. Secondly, D_{Oi} must be nondecreasing for successive increments. If $D_{O(k+l)} < D_{Ok}$, as could occur through consideration of very low dosages produced by the trailing edge of a cloud over an extended time period, it is recommended that $D_{O(k+l)}$ be set equa1 to D_{Ok} before proceeding to the next interval. Thirdly, since it is not apparent that the maximum value of D_{Oi} will always exceed the actua1 peak two-minute accumulation during cloud passage, a numerical comparison should be made, with the larger value obviously accepted as the basis for hazard-distance estimation.

ANNEX C

METHOD FOR CALCULATING RATES OF EVAPORATION FROM PUDDLES OF LIQUID TOXIC SUBSTANCES

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ANNEX C

METHOD FOR CALCULATING RATES OF EVAPORATION FROM PUDDLES OF LIQUID TOXIC SUBSTANCES

C.1. GENERAL

The general model for computing rates of evaporation from puddles of toxic substances is presented in this Annex. Its principal value here is to enable analysts to calculate evaporation rates for situations whose parameter values are out of the range of Figures 1, 2 and 3 in Section 3.4 of the Technical Paper. In particular, evaporation rates for toxic substances other than the three chemical warfare agents, GB, VX, and HD, may be calculated by way of this model. For completeness, input data used to compute evaporation rates for those three agents are also provided in Table C.1.

The evaporation-rate model described herein was adapted from the Chemical Engineers Handbook1, by Solomon2, for application to chemical hazard prediction problems. It is reproduced here as it was originally resented in ORG 40, with the exception that all units of measurement have been converted to the Metric system. The format is that of a “cookbook recipe” for deriving evaporation rates.

C.2. THE REYNOLDS NUMBER

Determine the dimensionless Reynold's number, N_{Re}, for the air flow from the equation

$$N_{Re} = \lambda \, . \, U \, .. \rho . / \cdot \mu \times 10^4$$

where

λ = downwind length of the puddle (m),

U = wind speed (m/sec),

ρ = density of the air (gm/cm^3),

μ = viscosity of the air (poise (gm/cm · sec)).

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[1] Perry, M.H. (editor), Chemical Engineers’ Handbook, 3rd Edition, McGraw-Hill Book Company, Inc., 1950.

[2] Solomon, I., et al, Methods of Estimating Hazard Distances for Accidents Involving Chemical Agents (U), ORG Report No. 40, US Amy Munitions Command, Operations Research Group, Edgewood Arsenal, MD, February 1970. CONFIDENTIAL.

The density of air in gms/cm^3 can be determined by

$$\rho = \frac{.35232}{T} \cdot P$$

where

T = temperature (^{O}K),

P = ambient pressure (atm).

The viscosity of air can be determined from

$$\mu = e^{(4.36 + .002844T)} \text{ x } 10^{-6}$$

C.3. THE MASS TRANSFER FACTOR

From the Reynolds number, calculate the mass transfer factor, j_m, as follows:

$$j_m = .0664 \, N_{Re}^{-0.5} \qquad \text{for } N_{Re} \leq 20{,}000$$

$$= .0366 \, N_{Re}^{-0.2} \qquad \text{for } N_{Re} > 20{,}000$$

C.4. THE MASS TRANSFER COEFFICIENT

The mass transfer coefficient, K_g, is calculated by

$$K_g = G_m \cdot j_m \cdot (\mu/\rho d)^{-2/3}$$

where

K_g = mass transfer coefficient (gm-moles/sec . cm^2),

G_m = molar mass velocity of air (gm-moles/sec . cm^2),

($\mu/\rho d$) = Schmidt number (dimensionless),

d = diffusivity (dimensionless).

The molar mass velocity of air can be determined by the formula

$$G_m = \frac{U \cdot \rho}{M_A} \text{ x } 10^2$$

where M_A = molecular weight of air 29 gms/gm mole

The diffusivity of air, d, may be computed from

$$d = .0043 \frac{T^{3/2}}{P\left(V_A^{1/3} + V_L^{1/3}\right)^2} \cdot \left[\frac{1}{M_A} + \frac{1}{M_L}\right]^{1/2}$$

where

T = temperature (^{O}K),

P = ambient pressure (atm),

V_A = molecular volume of air at normal boiling point (cm^3/gm mole),

V_L = molecular volume of liquid at normal boiling point (cm^3/mole),

M_L = molecular weight of liquid (gm/gm mole),

M_A = molecular weight of air, gms/gm mole.

The molecular volumes V_A and V_L can be determined from Table 10 in Section 8 of the cited handbook. For the three chemical agents whose evaporation rates are presented in graphical form, the necessary input data required for calculations is contained in Table C.1.

C.5. THE EVAPORATION RATE

The driving force for evaporation is the difference between the mole fractions of the agent at the agent-air interface and in the main air stream. If the mole fraction in the air is assumed to be negligible, the driving force can be approximated by the ratio of the vapor pressure of the agent (at the prevailing temperature) to one atmosphere in equivalent units, as shown in the following equation:

$$E = K_g \,.\, M_L .\, P_L \,/\, (760 \,.\, P) \,.\, 6.0 \,.\, 10^5$$

where

E = evaporation rate of liquid (gms/m^2 min),

P_L = vapor pressure of liquid at liquid air interface (mm Hg).

TABLE C.1. AGENT INPUT DATA

AGENT	MOLECULAR WEIGHT (gms/gm-mole)	MOLECULAR VOLUME (cm^3/gm mole)	VAPOR PRESSURE RELATIONSHIP (mm Hg)
GB	140.1	148.5	$\log P_L = 8.5916 - 2424.5/T$
VX	267.4	342.5	$\log P_L = 7.70897 - 3187.0/T$
HD	159.1	157.6	$\log P_L = 38.525 - 4500.0T - 9.86 \log T$

C.6. THE EVAPORATION RATE INTO STILL AIR

This methodology is to be used when the incident occurs within a closed building or other confined location that precludes the movement of air during the evaporation of the toxic liquid. The evaporation rate into still air is calculated using the following semi-empirical equation[1]:

$$Es = 292(1 + 0.51\, Re^{1/2}\, Sc^{1/3})\, \ln \frac{1}{1-P_v} \cdot \frac{M_L}{T} \cdot d \cdot \frac{\lambda}{2}$$

Where:

Es = evaporation rate (grams/min)
Re = Reynolds number (using a wind speed of .03 m/sec)
Sc = Schmidt number
P = ambient pressure (atmos.)
P_v = vapor pressure of liquid (atmospheres)
M_L = molecular weight of liquid
T = ambient temperature (^oK)
d = diffusivity of air (cm^2/sec)
λ = diameter of spill (meters)

With:

$$Re = \frac{0.03\, \lambda\, \rho}{\mu}$$

ρ = density of vapor (g/cm^3)
μ = viscosity of vapor (g/cm/s)

$$Sc = \frac{\mu}{\rho d}$$

---

[1] Rife, Richard. Calculation of Evaporation Rates for Chemical Agent Spills, Office of the Project Manager for Chemical Demilitarization and Installation Restoration, Aberdeen Proving Ground, MD. (Equation 17). October 1978

In calculating the Reynold's number, the effect of the agent vapors or the air viscosity and density will be ignored.

$$\rho = \frac{.3487}{T} \text{ (for water vapor pressure of 25mm Hg)}$$

$$d = \frac{.00205T^{3/2}\sqrt{\frac{1}{29} + \frac{1}{M_L}}}{P\,\sigma_{12}^2\,\Omega_D}$$

Note that this is equation 23 in Rife's methodology

Where

d = diffusivity (cm^2/sec)

$\sigma_{12} = \frac{\sigma_1 + \sigma_2}{2}$ = average molecular collision diameter (angstroms)

Ω_D = collision integral for diffusion

The value of Ω_D is evaluated using the following empirical equation:

$$\Omega_D = 1.075\left(T\frac{\kappa}{\varepsilon_{12}}\right)^{-.1615} + 2\left(10\frac{\kappa}{\varepsilon_{12}}T\right)^{-.74}\log\left(10\frac{\kappa}{\varepsilon_{12}}T\right),$$

where

$$\frac{\varepsilon_{12}}{\kappa} = \sqrt{\left(\frac{\varepsilon_1}{\kappa}\right)\left(\frac{\varepsilon_2}{\kappa}\right)}$$

The following agent parameters apply:

TABLE C.2. AGENT PARAMETERS

	ML	σ	Ɛ/k (^{O}k)
air	29.0	3.711	78.6
GB	140.1	6.25	521
VX	267.42	8.26	691
HD	159.1	6.37	593

The remaining intermediate variables use the same auxiliary relationships as for moving air conditions.

ANNEX D

METHODS FOR CALCULATING HAZARDS FOR EXPLOSIVE DISSEMINATION OF VX AND HD

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ANNEX D

METHODS FOR CALCULATING HAZARDS FOR EXPLOSIVE DISSEMINATION OF VX AND HD

D.1. GENERAL

This annex presents an interim method for computing the hazard distances associated with explosive dissemination of agents VX and HD.

Explosive dissemination of these persistent agents yields source clouds characterized by vapors as well as liquid droplets whose diameters span a considerable size range (i.e., from molecular diameters to thousands of microns). Thus, there are two types of threats from explosives involving those agents: (1) the percutaneous, or skin-absorption, threat due to the impaction of droplets on personnel, and (2) the respiratory threat due to inhalation of either the vapor or the aerosol.

Given that data existed to describe the particle size distribution in the aerosol, the settling velocities of droplet sizes in the atmosphere, and the efficiency of droplet impaction on personnel, the Generalized Prediction Model described in Annex A would be applied, incrementally, to the vapor and to each of several droplet size ranges in the aerosol. The results of those calculations would be summed at each point in the challenged area. The hazard distance associated with the combined vapor/aerosol threat would be specified as the required hazard distance. However, adequate data simply do not exist. Therefore, empirical methods were derived from analyses of test data. Those methods, originally described in ORG 40[13], have been simplified and adapted for use here. A complete description of the data base, and an explanation of this specialized methodology are presented on pages 140 thru 160 of ORG 40.

D.2. METHOD FOR VX

Figure D.1. shows the “1% lethality” hazard. distance, in feet, associated with the release of VX vapor and aerosol thru explosive dissemination. Each line shown on that figure represents a Pasquill stability category. Lines A and B represent lapse conditions, in which cases the predominant hazard arises from the percutaneous challenge. Hazards under conditions of neutral stability (i.e., C and D) and weak inversions (i.e., E) are also dominated by percutaneous effects. Maximum hazards under strong inversions (i.e., F) arise solely from the long-distance travel of the vapor under the inversion cap.

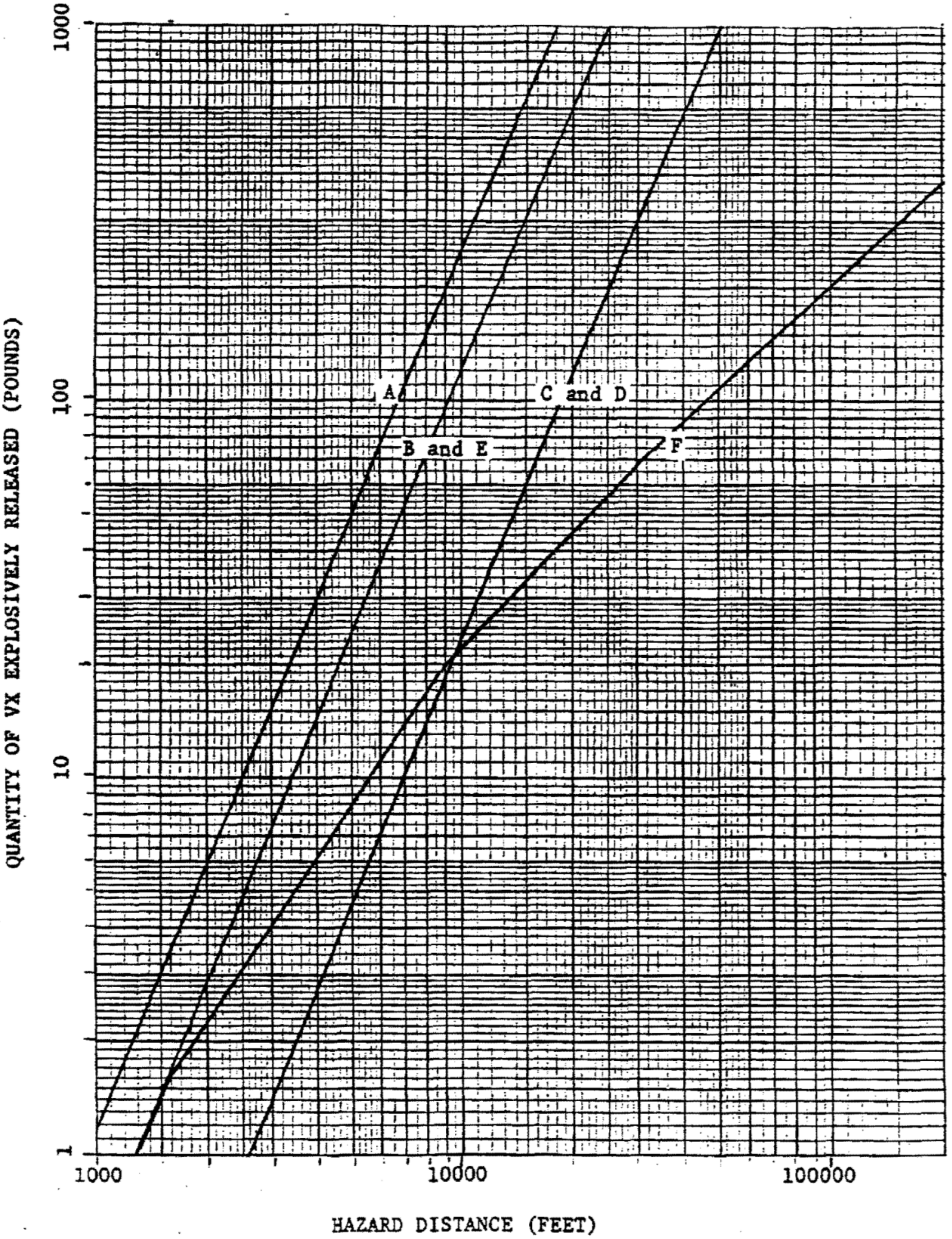


Figure D.1: Hazard Distance for Explosively Disseminated VX

Application of Figure D.1. to problems involving accidental explosive releases of agent VX is as follows:

(1) Determine the number and type of munitions involved in the explosive releases.

(2) Compute the total amount of agent released.

(3) Enter that quantity of agent (in pounds) into the ordinate scale in Figure D.1.

(4) Proceed across Figure D.1. to the appropriate meteorological stability category of interest. [The stability category can be determined from Table 1, 16.]

(5) Read the maximum credible hazard distance, for 1% lethalities, on the abscissa scale.

D.3. THE METHOD FOR HD

Figure D.2. and Table 9.1. must both be used to determine hazard distances associated with accidental explosive releases of agent XD. The method is as follows:

(1) The micrometeorologica1 conditions of interest (i.e., windspeed, temperature, and stability category) must be determined. Temperature may be estimated from historical data. Stability category and windspeed may be estimated from Table 1, page 16.

(2) Determine the fraction of agent airborne as vapors and droplets from Figure D.2. as follows:

(a) Enter ordinate M on Figure D.2. at the appropriate windspeed value.

(b) Construct a straight line from the windspeed on ordinate M, thru the correct temperature on diagonal N, to a point on ordinate P.

(c) From that point on ordinate P construct a straight line, thru the stability category on diagonal Q, to a point on ordinate R.

(d) From that point on ordinate R construct a straight line, thru the 4.2" Mortar mark on the diagonal, to a point on the ordinate S.

(3) Using the value of S determined in the previous step, compute the Final Reference Value from the following equation:

$$FRV = S\left(\frac{5}{U}\right)W,$$

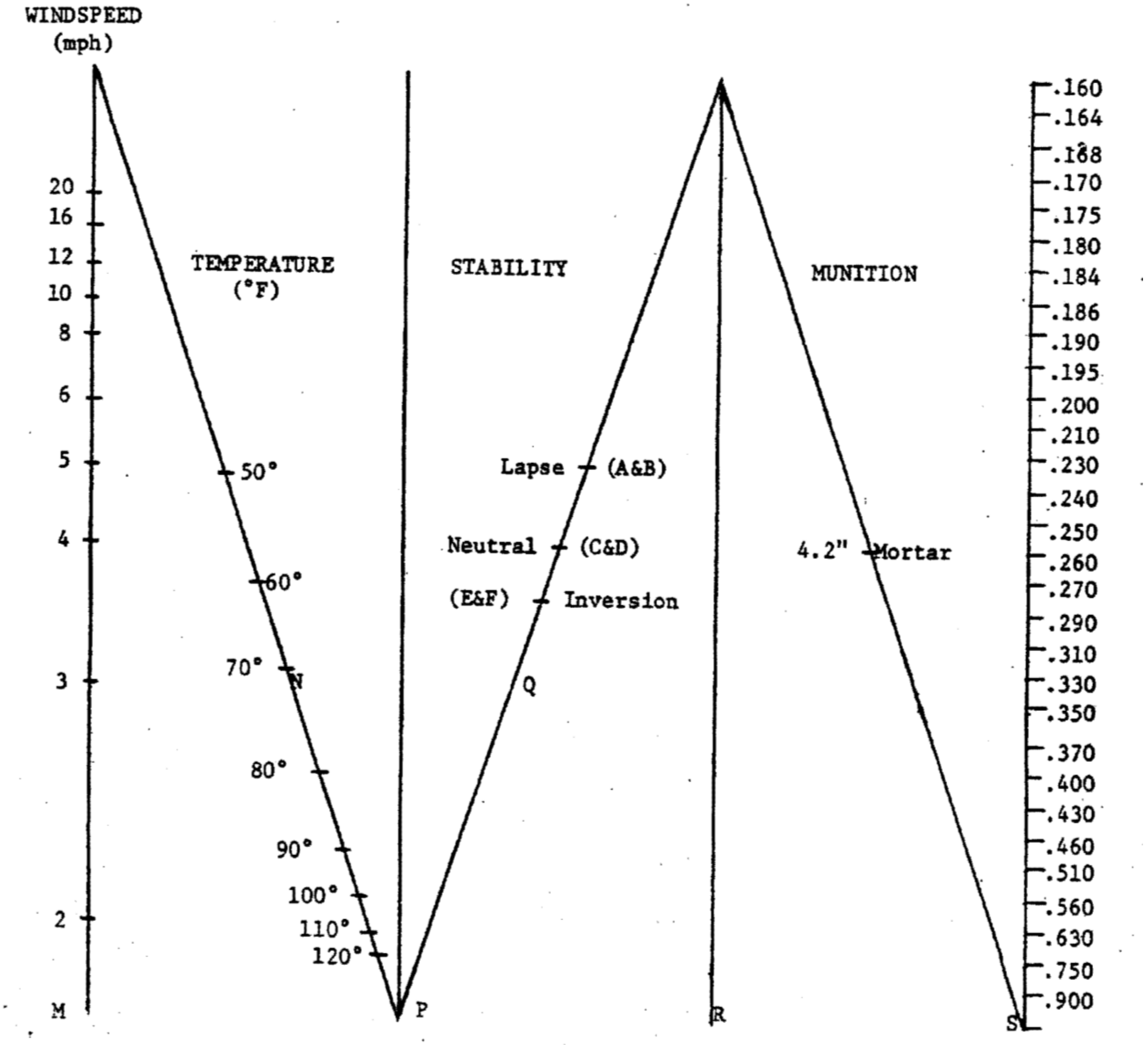


Figure D.2: Nomograph for Determination of the Final Reference Value for Agent HD where U is the windspeed (mph) estimated in Step 1 and used in Step 2. W equals 0.5 for the 105MM Howitzer projectile, 1.0 for the 4.2" Mortar, or 1.75 for the 155MM Howitzer projectile.

(4) The Final Reference Value is used together with the data in Table D.l. to determine the hazard distance, in feet , as follows:

(a) Enter Table D.1. on the line whose value is closest to the Reference Value calculated in Step 3.

(b) Determine the number of munitions involved in the accidental explosive release of HD.

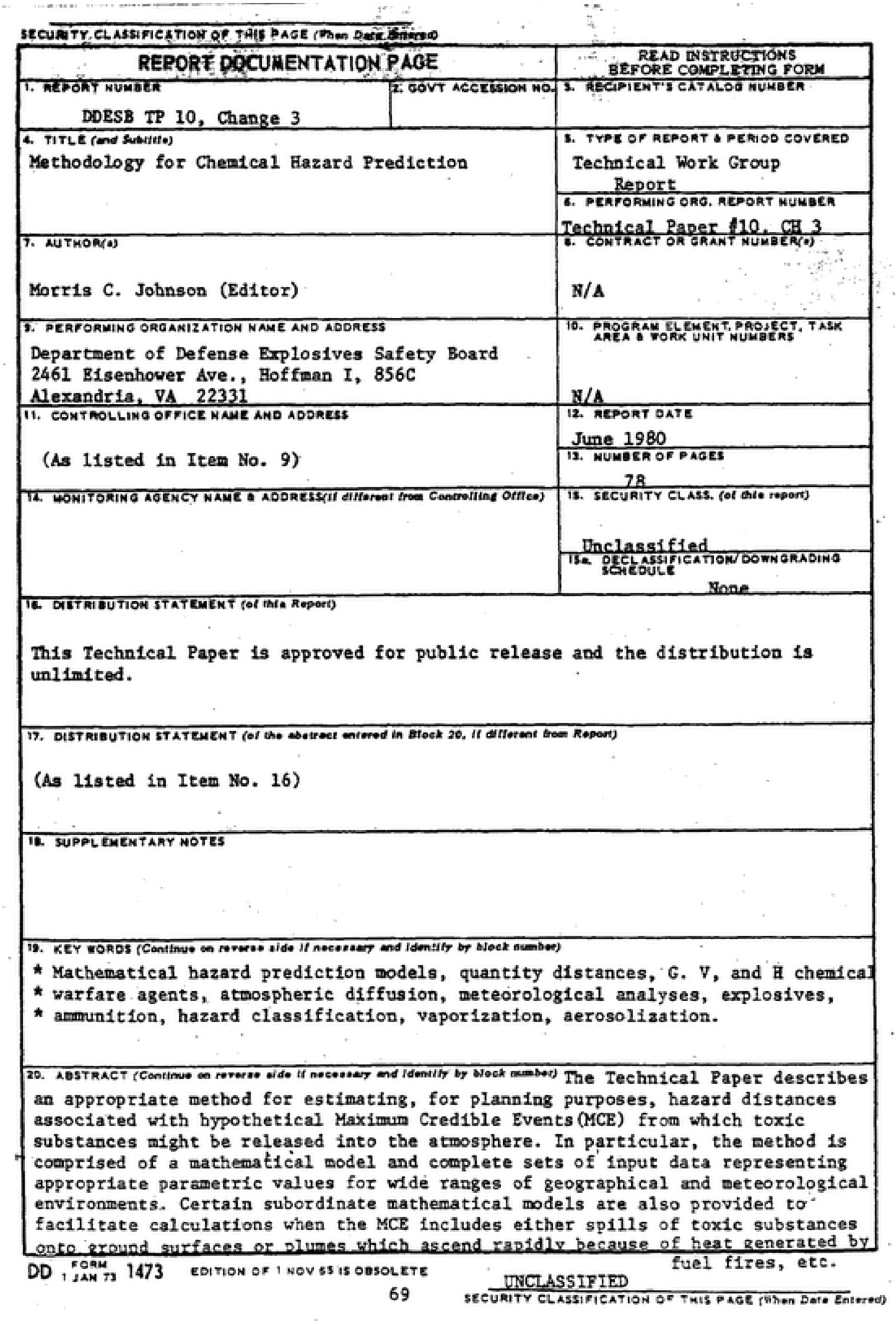
(c) Enter Table D.l. in the major column appropriate for the number of munitions involved. Select the stability subcolumn consistent with that determined in Step 1 and used in Step 4.

(d) Proceed down the subcolumn to the data line associated with the Final Reference Value as calculated in Step 3.

(e) Interpolate between data lines in the subcolumn, if necessary, to determine the hazard distance, in feet.

Table D.1. Hazard Distances (feet) for Explosively Disseminated HD

	NUMBER OF MUNITIONS INVOLVED IN EXPLOSIVE DISSEMINATION OF HD											
FINAL REFERENCE VALUE	1			2			5			10		
	L	N	I	L	N	I	L	N	I	L	N	I
.125	25	45	55	35	65	85	52	120	220	70	175	250
.250	35	65	85	45	105	135	70	17	250	85	250	400
.500	45	105	135	65	155	220	85	250	440	105	340	600
.750	55	130	180	75	190	280	95	300	500	120	420	750
1.000	65	155	220	80	220	325	105	340	600	130	460	850
1.250	70	170	250	85	250	400	110	390	650	135	520	970
1.500	74	190	280	90	275	430	120	420	750	140	560	1050
1.750	80	210	340	95	300	490	125	460	825	150	625	1200
2.000	82	230	360	100	320	540	130	480	900	155	650	1300
2.250	84	240	380	105	340	580	135	500	650	160	675	1400
2.500	86	250	400	110	360	600	140	540	1000	165	725	1500



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19. KEY WORDS (Continue on reverse side if necessary and identify by block number):

* Mathematical hazard prediction models, quantity distances, G, V, and H chemical
* warfare agents, atmospheric diffusion, meteorological analyses, explosives,
* ammunition, hazard classification, vaporization, aerosolization.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The Technical Paper describes an appropriate method for estimating, for planning purposes, hazard distances associated with hypothetical Maximum Credible Events (MCE) from which toxic substances might be released into the atmosphere. In particular, the method is comprised of a mathematical model and complete sets of input data representing appropriate parametric values for wide ranges of geographical and meteorological environments. Certain subordinate mathematical models are also provided to facilitate calculations when the MCE includes either spills of toxic substances onto ground surfaces or plumes which ascend rapidly because of heat generated by fuel fires, etc.

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